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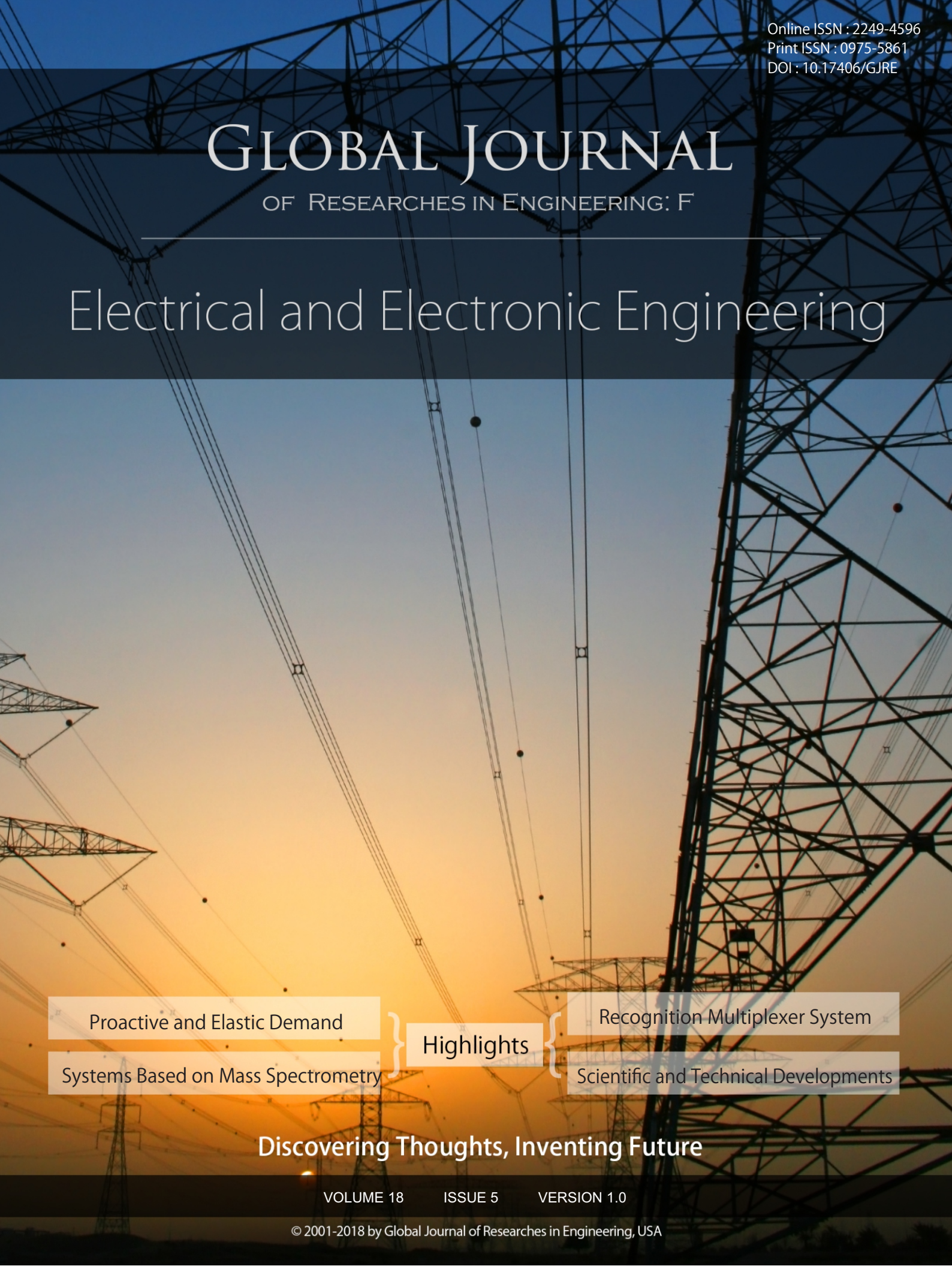

Proactive and Elastic Demand

Systems Based on Mass Spectrometry

Highlights

Recognition Multiplexer System

Scientific and Technical Developments

Discovering Thoughts, Inventing Future

VOLUME 18 ISSUE 5 VERSION 1.0

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New Scientific and Technical Developments in the Areas of Electronic Systems Based on Mass Spectrometry

By Aldan Sapargaliyev

Abstract- TOFMS and EEFE-MS (EEFE-MS - DSSSO and KUTP electronic systems based on TO mass and mass spectrometry) are now widely used in many fields of human activity. TOF MS made a decisive contribution to many breakthrough achievements of science, in particular, thanks to the use of mass analyzers of this type, the human genome and the genomes of other organisms were deciphered.

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Strictly as per the compliance and regulations of:

Новые научно-технические разработки в направлениях электронных систем, основанныхна масс-спектрометрии

Aldan Sapargaliyev

Принятие обозначения и сокращения:
ДСССО – диагностики структуры, состава, состояния объектов (веществ и живых организмов);
КУТП – контроля, управления технологическими процессами;
CGCS – обобщенно-потенциальное поле;
CO– корпускулярная оптика;
OSTT CO– общая пространственно-временная теория корпускулярной оптики;
TOFMS –времяпролетный масс-спектрометр;
R – Отражательный;
MR – многоотражательный;
nD – n- мерный, гдеn=2,3;

TOFMS и EEFE-MS (EEFE- MS – электронные систем ДСССО и КУТП, основанные на TOFмасс-спектрометрии) в настоящее время начали широко используются во многих сферах человеческой деятельности.

TOF MS внесли решающий вклад во многие прорывные достижения науки, в частности, именно благодаря использованию масс-анализаторов такого типа была выполнена расшифровка генома человека и геномов других организмов.

Предлагаемые нами принципиально новые концепции, технологии, теоретические и экспериментальные работы создают основу для быстрого продвижения по пути:

- **создания нового поколениясверхвыскоразрещающих, светосильных, компактных и с новыми функциональными возможностями различного назначения TOF MS и EEFE-MS и широкому использованию их во многих новых сферах, в частности в быту;**
- **контроля и управления любого технологического процесса, в частности для создания новых видов веществ и материалов с заданными свойствами и т. п.;**
- **контроля и диагностики состояния любого объекта, включая неживого и живого, в частности для медицинской диагностики, биологических исследований и т. п.;**
- **новых научных открытий в областях биологии и медицины, основные законы которых малоизвестны человечеству.**

Author: e-mail: oiarna.ass@gmail.com

I. Актуальные Проблемы Научно-Технического Развития Направлений TOFMS и EEFE-MS

В настоящее время показатели функциональных характеристик TOFMS и EEFE-MS весьма слабые, чем требуемые, связанные с проблемами биологии, медицины,контроля безопасности (качества и состава) пищевых продуктов, контроля и управления технологическими процессами при наличии органических веществ.

Во-первых, известныйна рынке "PegasusGC-HRT"(LECO Corporation,США, 2005 г.),один из видов MR TOFMS,выполненныйнаоснове, предложенной в 1992 году казахстанскимиучеными концепции«2D MRмасс-спектрометрии», имеетрекордное, среди TOFMS,длянастоящего времени разрешение – около4 5 000 (для300а.е.м.).

Для анализа органических веществ необходим TOF MS, с разрешением100тыс. и более. Вследствие ограниченных возможностей инструментариевCO, до настоящего времени онивторглисьвосновном- внежив-уюприроду,причем,тольковобластьнеорганическихвеще ств. Для широкого вторжения в областииссле-дования органическихвеществ и живой природы –большойи-важнейшейсоставляющейпланетыЗемля, нео-бходимо разработать революционно новое поколение инструментариев CO, одним из которых является TOF MS.

Во-вторых,весьма ограничены возможностиод-но-временного многокоординатного анализа по объему.Все процессы развиваются в зависимости от времени, а также в объеме изучаемого объекта с изменениями в пространстве (следствие процесса распространяется в пространстве). В частности, чтобы корректно контролировать и управлять процессами в веществах и живых объектах, особенно быстропр-отекающими процессами, необходимо одновременно контролировать (определять ход процесса) в различных точках.

В настоящее время, все известные MS, кроме их параллельно-многоканальных квадрупольных видов, являются одноканальными канально-однотрактными и выполнены с обеспечением возможности одновремен-ного анализа только однотрактного ионного потока. Многоканальная,канально-однотрактнаясистема квад-рупольных MS, как и все известные одноканальные MS

с квадрупольной ионной ловушкой обладает: малым *диапазоном*регистрируемых *масс;* невысокой точностью определения массы – < 20 ppm, низкой величиной соотношения разрешение/себестоимость.

*В-третьих,*у TOF MSотносительно невысокие-светосилаи трансмиссия.

II. Предпосылки К Нашим Новым RESEARCH, AND INNOVATION Работам В Направлениях CO, И Времяпролетноймасс-Спектрометрии

Известные основы концепции теории механики CGCS (CGCS – обобщенно потенциальные поля), а также один из его важных разделов CO(CO – corpuscularoptics) содержащиеся современных учебниках технических ВУЗов всего мира, построены более чем 100 лет назад[1].

Казахстанские ученые,начиная с восьмидесятых годов 20-го века,внесли и вносят большой вклад в развитие теории CO.

- ✓ В восьмидесятых годах 20-го века, разработали новый математический метод – метод центральной частицы (автор основных идей и руководитель работ Якушев Е.М.), решив математическую проблемуописания физических процессов в области с особыми точками при движении частиц в них,и создали современную общую пространственно-временную теорию корпускулярной оптики (OSTTCO). Основные результаты этих работ изложены Сапаргалиеым А.А в 1987 г. в его диссертации[11] на соискание степени доктора физ.-мат. наук и в обзорных статях[9]-[10]Якушева Е.М., написанные по предложению и при поддержке редакции международного журнала «Advancesin ElectronicsandElectronPhysics».
- ✓ На основе OSTT CO,в 1985 г.Сапаргалиевым А. А. предложен и 1987 г. под его руководством был созданопытно лабораторный образец оригинального TOF MS-FTAс фокусировкой кольцо-кольцо и впервые в мире была экспериментально осуществлена пространственно-временная фокусир овка ионного пакета с помощью неоднор одного (безсеточного) электростатического отраж ающего поля (ионного зеркала). TOF MS-FTA был усовершенствован в 1990 году.Результаты этих работ изложены в докторской диссертации[11]и в отчете по научно-исследовательской работе[12].
- ✓ Этиработы впервые экспериментально подтвердиливыводыOSTT COи открылиперспек-тивыдальнейшегоразвитияинструментариевCO.Отметим также, что сегодня, практически ,всеинс-трументы-COсоздаютсяснеоднородными полями (без сеток).
- ✓ В 1992годуЛ.М. Назаренко, Л.М. Секунова иЕ.М. Якушев предложили (SU1725289 A1, A.C.) высокоразрешающий 2DMRTOF (2DMRTOF – двумерный многоотражательный времяпролетный масс-спектрометр) с время-пространственной фокусировкой, где особые точки расположены в одной плоскости (в 2-мерном пространстве). В настоящее время наиболее высокое разрешение, около 45 000, среди известных на мировом рынке TOF MS, имеет "PegasusGC-HRT"(LECO Corporation,США), техническое решен ие и теория которого, созданы казахстанс кими специалистами в SU1725289 A1, A.C..
- ✓ В2010г.на основе OSTT COпредложена (SapargaliyevA. A. US 8,598,516 B2 и др.) конц еп ция«3D5Rмасс-спектрометрии»,втомчисле(a)3D-5R R(Multi-Reflector);(b)концепциюMultipathмасс-спект рометрии;(c)новыевидыкорпускулярно-оптиче ски хэлементовиустройствдляреализациипредложенных концепций. Концепция«3Dмасс-спект рометрии»пр едоставляетпринципиальноновыевозможностидляра звитиямасс-спектрометр ии, посравнени юсдругим иизвестнымиконцепциями. Наосновематематическ ого и компьютерного моделирования показано, что системы 3D масс- спектрометрии могут одновременно обладать многократно превосход ящимразрешением (внесколькосоттысяч) ичувств ительностью,ибытьболеекомпактным,чем лучшиеиз вестныеаналоги. Упомянутаяконц епция Multipath (многоканального)MSмногократноповышаетпроизво дительностьработыMS, достоверностьполуче ннойсе гопомощьюинформациииприводиткновымфункцион альнымвозможностяммасс-спектрометрии.
- ✓ Теоретическиеисследования под руководством Якушева Е.М.,проведенные в 2005-2013 г.г. нао с н овеOSTT CO,(например[10],) ,определилипринципи альныепути создания нового вида теневого CO микроскопа и увеличенияразрешениеэлектро нных микроскоповнадвапорядка (100 раз), по сравнению с известными в мире аналогами.

В настоящее время «метод центральной частицы», OSTT CO и ихзначимостьприобрелиобще мировоепр изнание. На их основе в мире построены множество уникальных CO систем, которые внесли значительный вклад в прогресс человечества.

III. Предлагаемые Нами Новые Концепции/Технологий и Их Научно-Технические Решения

Для повышения разрешения, светосилы и функциональных характеристик масс-спектрометрии нами предложены ряд новые концепций/технологий[15]-[18] и разработаны научно-технические решенияих практической реализации:

- nD5RTOF(nD – n-мерная, 5 –петлевая,R – отражательная) масс-спектрометрия, в том числе 3D 25MRTOF(25-двухпетлевая, MR–многоотражательная) высокоразрешающая и сверхвысокоразрешающаямасс-спектрометрия, где n=2, 3;
- Pj(Pj–многотрактнаяили многокоординатная) масс-спектрометрия, где j>1 – количество трактов

- Fk (Fk–светосильнаямногосвязно-кроссоверная-масс-спектрометрия, в том числеэнерго-фильтровая, где k>1количество связи многосвязнного сечения ионного тракта,выполненная с обеспечением возможности отбора потока ионов на время-пролетное детектирование с заданной или регулируемой областью (выбора энергетической шириной и положения этой ширины) энергетического распределения ионов в потоке.При этом, по меньшей мере, один MS-канал выполнен энерго-фильтровым:
  (a) с предварительнойэнергофильтрацией(энерго-фильтрацияпри выходе из предварительно-формирующего блока перед анализаторным каналом)
  (b) с после дисперсионной энергофиль трацией (энерго-фильтрацияпоследисперсиивана лизато рноом канала и перед детектором).
- 3DS/TOF-F (S/TOF-F – ступенчатая времяпр олетная масс-спектрометрия (поэтапно времопр олетной фокусировки), выполненные с одной или более поверхностями эффективного отражения и одним или более отклоняющими и фокусиру ющимиэлементами.

В зависимости от состава отражателей, отклоняющихи фокусирующих элементов и их расположения, представители, 3DS/TOF-F делятся на несколько семейства.

3D5RTOFMS,выполненныена основеконцеп ии3 D5RTOFмасс-спектрометрии,по принципу работы делятся на три подтипа.

1) однопроекционно-двухпетлевидные3D5RTOF, (вви де 3D5ℓRTOFMS), выполненные с двумя или более поверхностями эффективного отражения (двумя или более линейными ионными зекалами);
2) многопроекционно-двухпетлевидные3D5RTOF, (в виде 3D5rRTOFMS), выполненныес одним или более криволинейными поверхностями эффективного многоотражения (с одним или более кольцевидными отражательными ионными зеркалами). Представители 3D5rRTOFMSделятся на два рода – круглой или многоугольной поверхностями эффективного многоотражения;
3) ступенчато- времяпролетные3D5RTOF(в виде3D 5S/TOF-FMS) выполненные с двумя или более поверхностями эффективного отражения и с одним или болеотклоняющими и фокусирующими элементами.

IV. Основные Технические И Коммерческие Преимущества Новых Концепции/Технологий И Их Научно-Технических Решенийперед Известными Аналогами

Недостатком 2DMRTOF-концепции является то, что усреднённая траектория потока ионов лежит в одной плоскости, при этом в этой плоскости линейное ионное зеркало не оказывает фокусирующее воздействие на поток ионов. Это приводит к тому, что для разделения, падающего в ионное зеркало и отраженного от него потока ионов, необходим значительный угол отражения α (рис. 1). При этом, как следует из рис. 1, после каждого отражения поперечная энергетическая дисперсия расширяетширину (эффект “хроматического размытия”) ионногопотокаи после N отражений величину суммарного расширения Δh_N ио нного потокаможно представит в следующем виде:

$$\Delta h_N \approx N(\Delta s_\varsigma)\sin\alpha \qquad (1)$$

где:

- стрелки показывают направлений движения ионного потока.
- h_ς – расстояние между двумя плоскостями $S_{\varsigma 1}$ и $S_{\varsigma 2}$ эффективных отражений ионов с различными начальными энергиями,
- Δs_ς –эффективная ширина потока ионов с различными начальными энергиями в области его отражении в ионном зеркале.
- N – количество отражения.

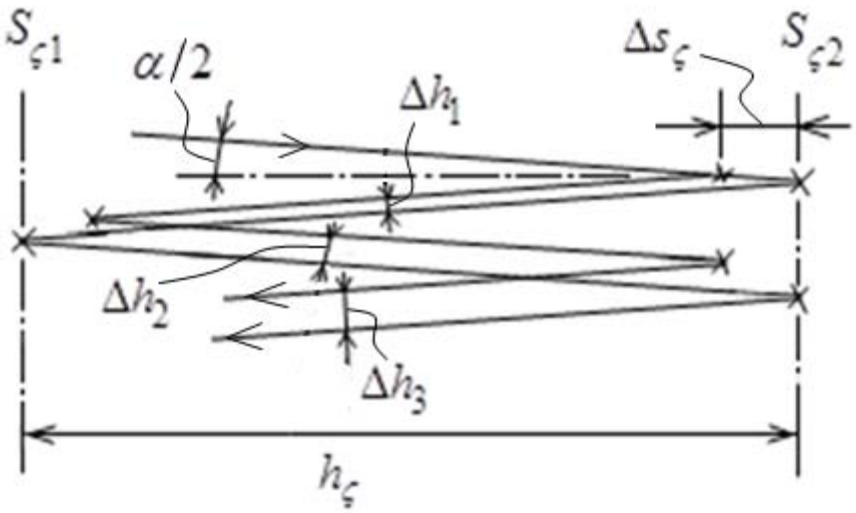


Рисунок 1: Эффект “хроматического размытия”, характерный для 2D MR TOF-концепции, в частности для “Pegasus GC-HRT”

Как показывает выражение (1), после нескольких отражений ширина размытия потока ионов Δh_N возрастет настолько что, дальнейшее удлинение траектории ионов не имеет смысла. Это ограничивает разрешение TOFMS, построенных на основе 2DMR-концепции. К тому же, при значительном количестве отражений, высота анализатора по вертикальной плоскости будет весьма большой.

В настоящее время 2DMRTOFMS создаются компанией Leco, США, под названием “Pegasus” по 2DMRTOF-концепции и имеет ограниченноеразреш ение, около 45 000.

Фокусировка потока ионов с помощью ионно-оптических линз после каждого отражения потока ионов, предложенная US No. 7,385,187 B2, не привели к улучшению разрешающей способности PegasusGC-HRT. Промежуточные ионно-оптические линзы порож дают, хаотические и, в принципе, неустранимые времяпролетные аберраций.

На рис. 2показаназамкнутаядвухпетлевиднаяп ро- екционная характернаяформатра ектории потока ионов в 3D∇2RTOFMS.

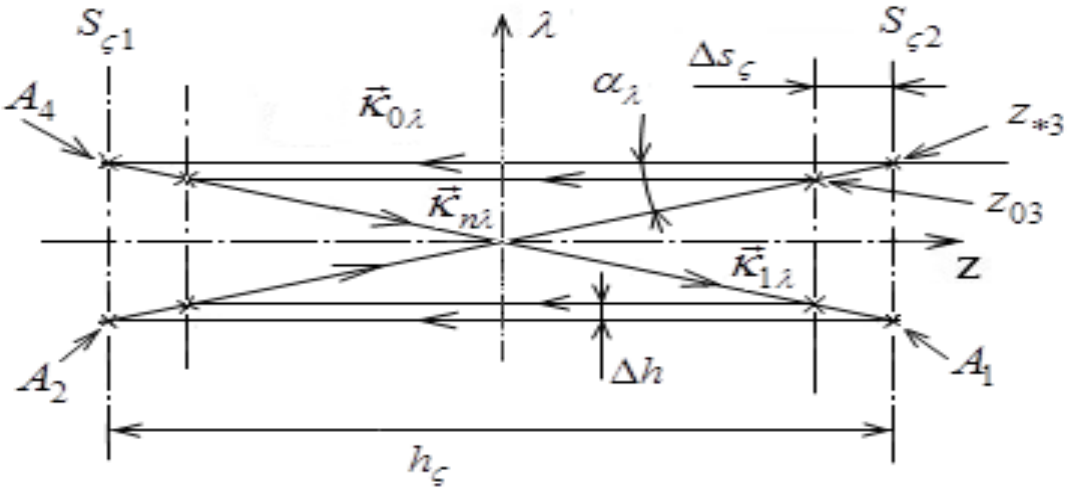


Рис.2: двухпетлевиднаяпроекционная характерная форма траектории потока ионов

На рисунке 2 введены обозначения параметров:

λZ – плоскость двухпетлевидностипроекционной характерной формы траектории потока ионов;

A_j – вершины эффективного отражения, где $j = 1, 2, 3, 4$;

$K_{1\lambda}$ *и* $K_{n\lambda}$ -единичные векторы, показывают направления движения потока ионов;

Δs_ς – эффективная ширина потока ионов с различными начальными энергиями в области его отражении в зеркале.

Главным достоинством nD5RTOF-концепции являются то, что, по меньшей мере, в одной из плоскости проекционная характерная форма траектории потока ионов является однопетлевым или двухпетлевым и в этой проекционной плоскости отсутствует эффект "хроматического размытия" потока ионов.Это связно тем, что после каждой пары антисимметричных отражений потока ионов, происходит взаимная компенсация ширины "хроматического размытия потока ионов Δh, образуемых при каждом из этих отражений. Это свойство nD5RTOF-концепции дают ей уникальные свойства, включая компактность и высокое разрешения по сравнению с другими концепциями.

Чтобы представить некоторые сведения об отдельных технических решениях вышеизложенных концепций рассмотрим только некоторые предстателей TOFMS.

a) 3D 25r MRTOFMS сверхвысокого разрешения (3D 25r UHR MRTOFMS)

Концепция основанная на 3-х мерном многоотражении ионных пакетов и обеспечивают увеличения разрешения, за счет большой времяпролетной дисперсии по массе ионов в сочетании с высокого порядка времяпролетной фокусировкой по разбросу энергии ионов. Увеличение времяпролетной дисперсии по массе ионов реализуется на основе увеличения длины пути и времени прохождения ионов в анализаторе3D 25MRTOFMS. Представители 3D 25 UHR MRTOFMS-будут иметь малые габариты и высокие разрешения, чем известные TOFMS.

Сверхвысокого разрешения 3D 25rUHR MRTOFMS является одним из типовсверхвысо коразрешю-щих 3D25TOFMS, который по виду отражателей и по принципам работ делятся на три подтипа.

1) 3D 25ℓ UHR MRTOFMS – однопроекционно-двухпетлевые, выполненныес четырьмя линейными ионными зеркалами, расположенные на вершинах правильного четырехугольника;
2) 3D 25rUHR MRTOFMS – многопроекционно-двухпетлевые, выполненные с двумя симметрично расположенными кольцевидными многоотражат ельными ионными зеркалами; Предста вители 3Dm5rMRTOFMSделятся на два рода – круглой и многоугольной поверхностями эффективного многоотражения;
3) 3D UHRS/TOF-F– однопроекционно-двухпетлевые, выполненныес четырьмя линейными ионными зеркалами и восемью цилиндрическими конден саторами.

Чтобы представить некоторыесведения об технических решениях3D 25 UHR MRTOFMS, на рис.3-5схематический показаны3D25rHRT MRTOFMS в проекции на горизонтальную (рис. 3 и 5) и на вертикальную плоскость (рис. 4):

- кругло-граничный 3D25r HRT MRTOFMS(рис. 3);
- n -гранено/секторно-граничный (многоугольный) 3D25r HRT MRTOFMS, секторные эффективные поверхности, отражения которых расположены вокруг одного центра (рис. 4).

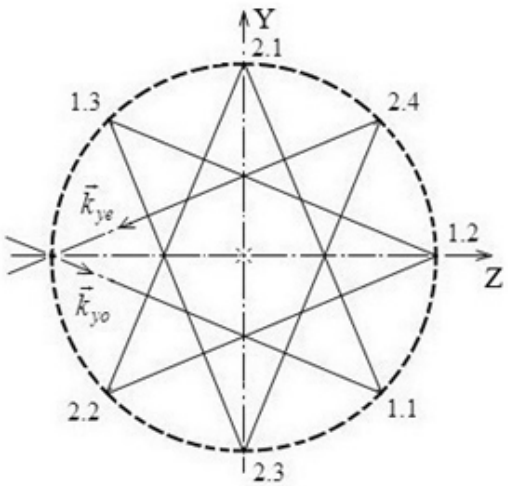


Рис. 3

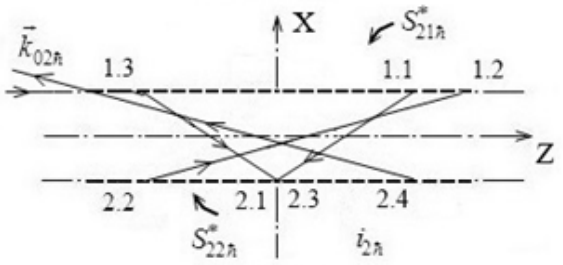


Рис. 4

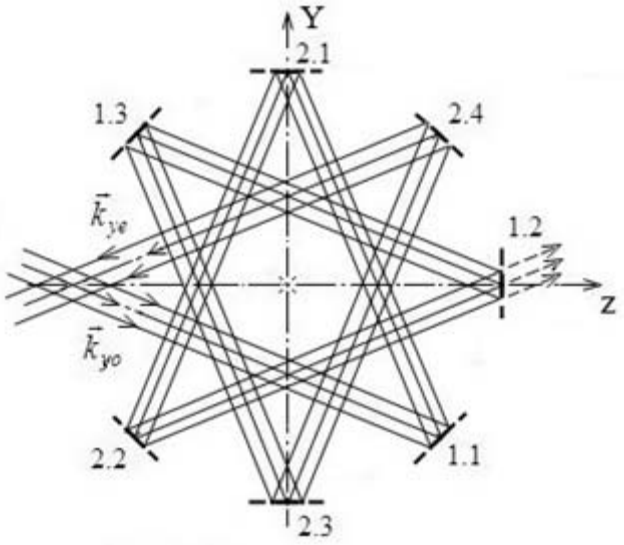


Рис. 5

На рис. 5 показана семиугольная отражающая поверхность. Конечно, на количество углов многоугольника нет ограничения. Многоугольная отражающая поверхность позволяет пропускать широкие ионные потоки.

Результаты математического и компьютерного моделирования 3D 25ℓR UHR MRMS доложены на международной конференции[14] и опубликованы на нескольких научных журналах. Они показали, что 3D 25ℓR UHR MS может одновременно обладать многократно превосходящимразрешением(внесколько-соттысяч) ичувствительностью,ибытьболеекомпактным (2 и боле раз), чем лучшие известные аналоги, например, PegasusGC-HRT.

Создан опытно лабораторный образец, который подтвердил исходные теоретические расчеты и перспективность выбранного нового научно-технического направления. (www.OiArna.com; /(https://drive.google.com/file/d/0B47EiWNeAC2qMzlhSlNuNndCTU0/ view?usp=sharing).

V. Высокоразрешающие Multipath Или Канально-Многотрактные (Несколько Ионных Трактов В Одном Канале) Ms (Ms-Pj)

Упомянутая концепцияMultipath(многотрактного) масс-спектрометр-ии многократноповышаетпроизводительностьработы MS, достоверностьполученной сегопомощьюинформ-ацииприводиткновымфункциональнымвозможностяммасс-спектрометрии.

Например,однимизперспективныхприложенийупомянутойконцепции с новыми функциональными возможностями,являетсяiKnife (IntelligentKnife,http://en.wikipedia.org/wiki/Iknife),разрабатываемыйWatersCorp.iKnife–этоинструмент, способный анализироватьчеловеческуюткань вреальномвременивовремямедицинскойоперации.Наосновемасс-спектрометриибыстройиспарительной ионизации(REIMS,http://www.chemport.ru/datenews.php?news=3584),iKnife,будучиинтегрировансостандартными электрохирургическимиинструментами,наосновесобранногоипроанализированногодыма,способенмгновенноопределитьстатусвырезаннойткани.

На рис. 6-8 показаны некоторые примеры возможных видов, на поверхности сечении, многотрактного ионного потока, где, соответственно j = 4, j = 6 и j = 2, гдеj – количество трактов.

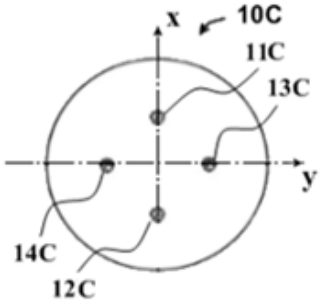


Рис. 6

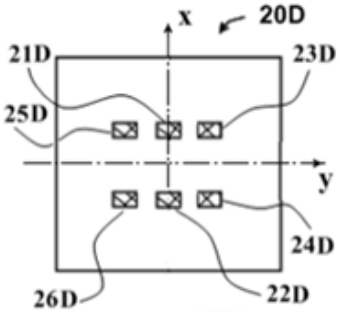


Рис. 7

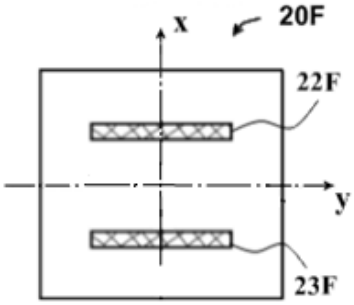


Рис. 8

Наиболее простыми видами выполнения канально-многотрактныхотражательныхRMS-jP, пред ложенных нами, могут бытьодноотражательны йRMS-Pjc одним линейным зеркалом и двуотражательный петлевой MS с двумя линейными зеркалами.

Предложенные нами многотрактныеRTOFMS-Pj обладают: с широким *диапазоном* регистрируемых *масс;*высокой точностью определения массы – < 3 ppm; высокой величиной соотношенияразрешен ие/себестоимость (например, более чем четыре раза по сравнению с тремя параллельными квадрупольными масс-спектрометрами).

b) *Светосильная многосвязно-кроссоверная MS(MSFk) с энергофильтрацией, где k>1*

Основные достоинства MSFk, выполненные с обеспечением возможности пропускания потока ионов на времяпролетное детектирование с заданной или регулируемой областью (выбора энергетической шириной и положения этой ширины) энергетического распределения ионов в потоке (энергофильторно-, MS-канал):

MSFkобладает до 3-х раз большей светосилой, чем его аналоги с ионным потоком центрально йодносвязаннойповерхностью сечения круглый формы, при его диаметре равный ширине многосвязной поверхностью сечения ионного потока.

MSFkс энергофильтрацией (с энерго-фил ьтровой диафрагмой в области кроссовера ионного потока) позволяет существенно повысить егоразреш ение.

Наибольший интерес для схемы TOF MSFkпредоставляет зависимости его разрешающей силы и трансмиссии/светосилы от ширины энергети ческого распределения (распределения количества ионов в зависимости от энергии ионов, см. рис.9) проходящей части ионного пакета (заштрихованная область под кривой распределения при температуре 20^0 С) из источника, через диафрагму.

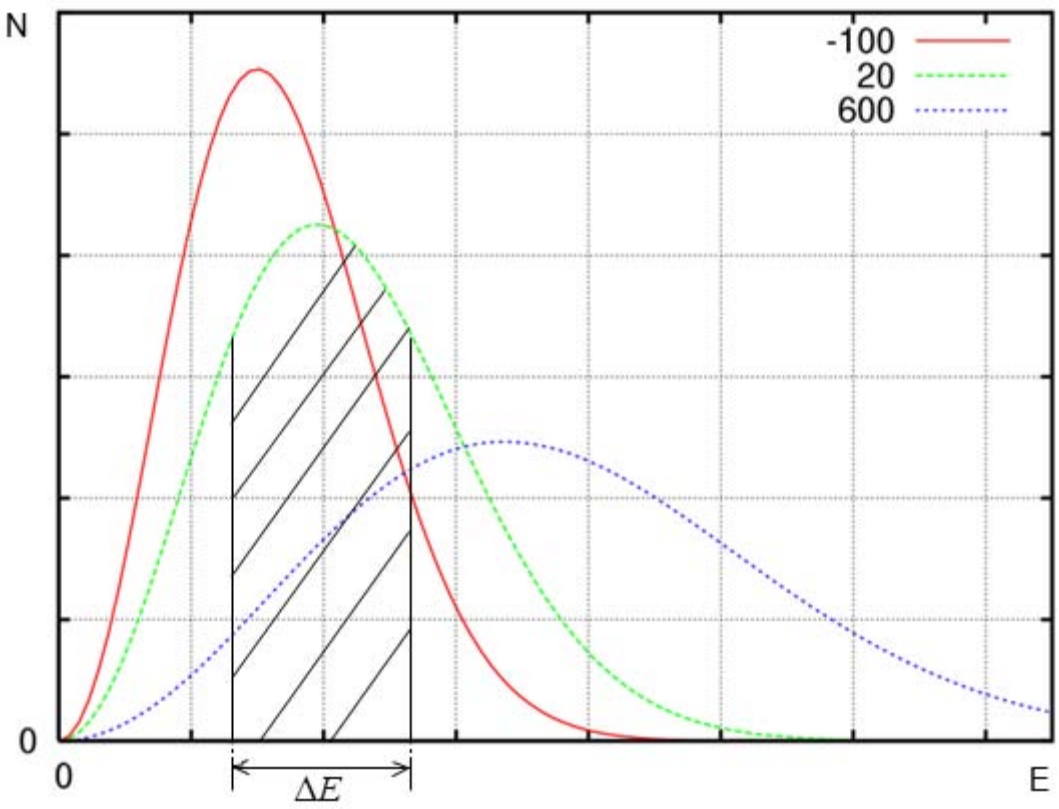


Рис. 9

На рис. 10, 11 и-13 показаны некоторые примеры возможных видов, двухсвязанных, на поверхности сечениия, ионного потока.Они могут быть использованы в TOF MSFk. соответственно: на фиг. 10–сдвумернойсимметриейраспределения поля;на фиг.10 и 11 – с любым изтрансаксиальной и двумернойсимме триейраспределениями поля;нафиг. 12– свращател ьной симметрией распределения поля.

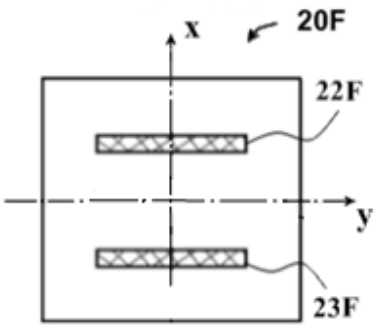


Рис. 10

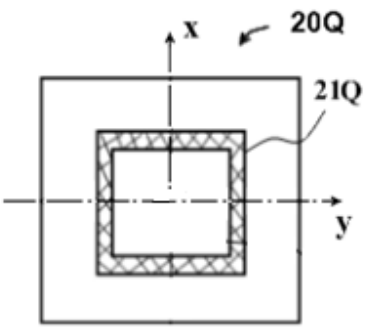


Рис. 11

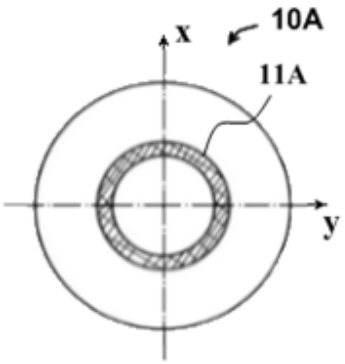
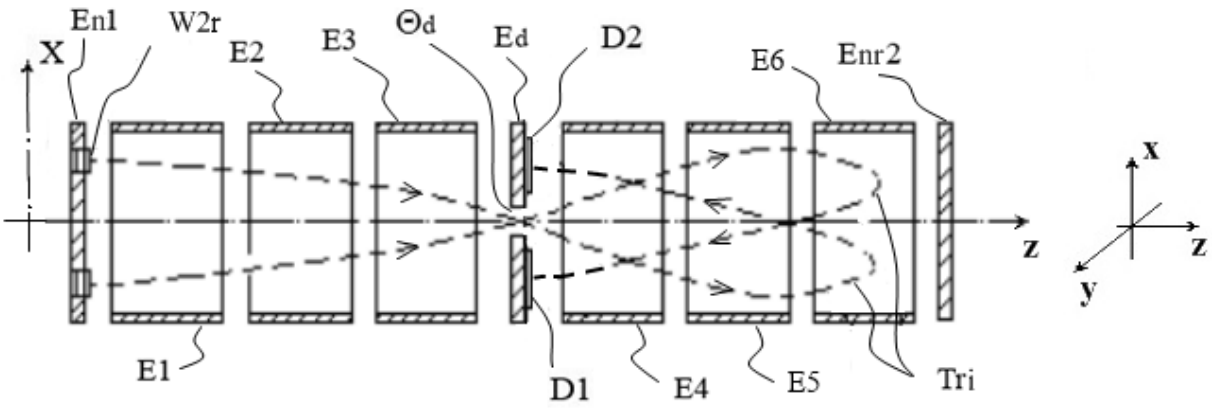
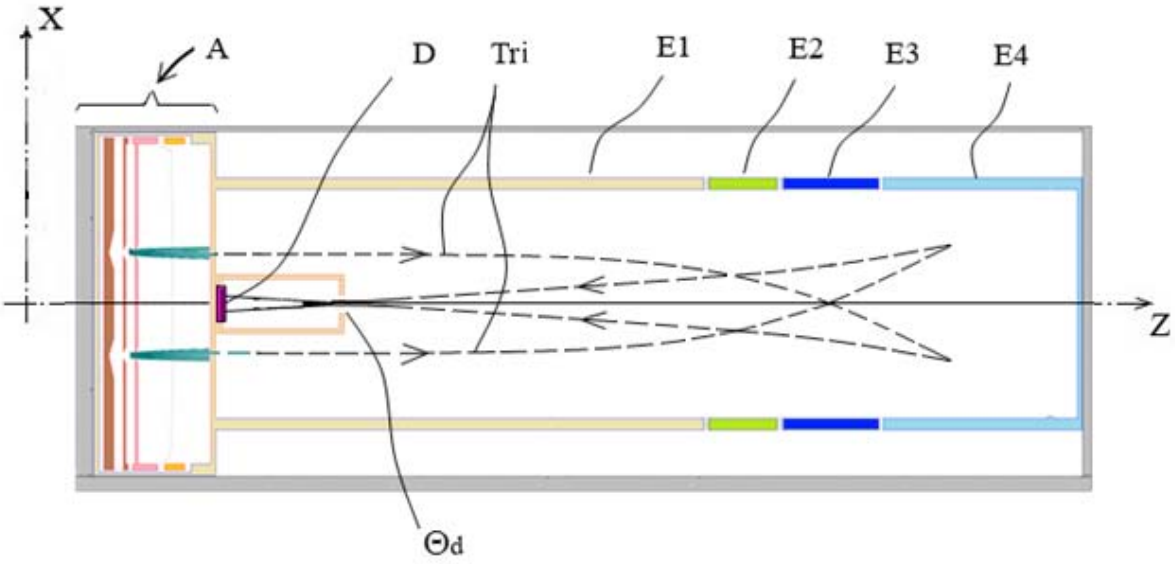


Рис. 12

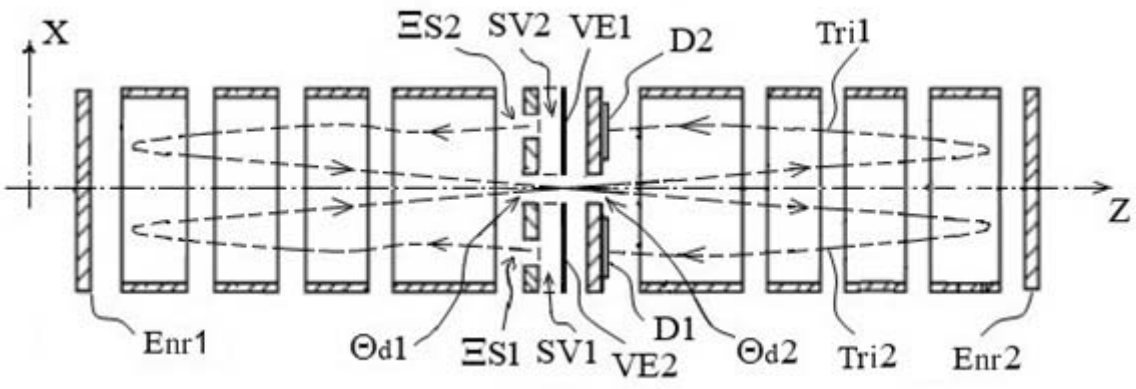
На рис. 13-15схематический представлены некоторые примеры выполнения TOF MSFk, где пунктирными линиями показаны траекторий ионов в анализаторе, стрелки на них показывают усредненные направлений движений ионов.



ФИГ. 13



Фиг. 14



Фиг. 15

Все технологические решения защищены.

VI. Маркетинг. Рынок Ежегодного Потребления Продукции MS

Согласно исследованию конкурентной среды, в 2010 году рынок ежегодного потребления мировой промышленности аналитических электронных систем составил около $40 млрд. с регистрируемым за прошлые годы ростом на 7% [19].

По сведениям крупнейшей исследовательской компании рынка MarketsandMarkets, рынок масс-спектрометрии оценивается в $4,9 млрд. в 2015 году и достигнет $7,3 млрд. к 2020 году со среднегодовым темпом роста в 8,1%[20].

С ростом требований общества к безопасности, улучшением потребительских качеств товаров и пищевых продуктов, спрос на аналогичные приборы и оборудование будет интенсивно расти.

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Deep Learning Algorithm for Speech Recognition Multiplexer System Suitable for World Congress Discussion

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Abstract- The difficulties encountered in building an intelligent speech recognition system and identifying various accents in speeches has been examined by this research.

The research has adopted the MFCC extraction techniques using the energy values in the spectrogram generated by the neural algorithm. The sampling procedures ensured that 1/16000 wave amplitude of a second intervals were enough sample size for speech to be recognized.

The deep learning neural network architecture is of 5- 9-6-3 configuration coded in python functional programming language with 250 epoch runs, while the back propagation method of iteration is used to ensure that the errors are brought to the barest minimum, with average value of about 0.002 0r 0.2% which is okay for training model.

The system as a whole is designed as a multiline multiplexer suitable for holding international congress meetings.

The MFCC extraction techniques showed that the energy values can be used by the neurons to recognize the usable pitch in a complex sound clips.

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I. Introduction

The Speech recognition in recent times has proved it's' efficacy in all our day to day activities, its' almost invading our lives, every individual has directly or indirectly has interaction with it. It's built into our mobile phones, game consoles, smart watches and all Digital Signal processing machines. It is the tool we use to interact with robots, though it's not a new field of endeavor, it has been around for decades, but the field is gaining acceptance and recognition in present times. There is need for Engineers and Technologists to embrace this technology for accurate Speech recognition in certain environments. Speech recognition accuracy lies in the bosom of deep learning, which makes it possible to predict accurately with almost 95% confidence when we interact with computers. This is achieved simply in this research by feeding the sound recording into the neural network and training it to produce the text and the owner of the voice. The research also intends to look into certain difficulties encountered when designing a system that recognizes speech since certain factors; such as the speed in speeches, which determines the mode of speaking and it varies from human to human [1], the research will try to examine this by using some kinds of extraction and processing techniques in addition to the deep learning neural network. In the study conducted by Vibha Tiwari, he examined that the property of speech signal can change as a function of time, and he used the MFCC extraction method to study the properties of signals such as energy, zero crossing, and correlation [1]. In a similar research on voice recognition algorithm using MFCC by Lindasalwa et.al, it was established that human voice conveys much information such as gender, emotion, and identity of the speaker, the research then used the tool of MFCC techniques to solve the problem of recognition which is based on human hearing perceptions that is limited to 1kHz. The MFCC was then used to study the variations of the human ears' critical bandwidth [2].

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II. Methodology

The model was designed for the purpose of recognising when a particular speaker is on board, so that other participants in a meeting can listen to the contributions of that particular speaker, the algorithm is also designed to recognise the country where the speaker is from, since each country from the meeting has been coded with a particular frequency range which is unique to that particular speaker. Immediately after his or her contributions, the deep learning can now give access to the others for their contributions, thereby acting as a multiplexer, giving access at a time during the speech and denying others for a while.

a) The Coding procedures

The current speaker making a speech is recognized by the machine as having a high value which is coded with digit 1, while as at that time the other speeches from the prospective Speakers are regarded as low value, with code 0, that is the speech of an accessed Speaker is given a priority as high value, while others are given low values and the machine will deny them an access.

The network Architecture assumed a continuous variable of vocabulary size.

b) The Soft Computing Requirements and Development

The soft computing aspect of the system involves; Speech recognition algorithm, Neural network building and integration of program segments. The system is coded using python functional programming language. The neural network used is a four layered neurons with two separate hidden layers of order 9 and 6 respectively before the output. The neural training employed is back propagation algorithm, to ensure that errors are computed through the sigmoid functions and brought to the barest minimum to recognize a speech.

c) The Model Conception

The research tries to model a speech recognition system using the properties of a sine wave and the energy values relating to the amplitudes of the wave. The system used the efficacy of Fast Fourier transforms to obtain the Spectrogram which contains the full sound clip. The results from the energy equivalent $E = 2A^2$ were introduced into the neural network to carry out the machine learning processes in other to give an output which is to recognise what the speaker is trying to say and the speaker. The Speech recognition algorithm was design using the MFCC extraction techniques which is based on human hearing perception. The amplitude of a wave is related to the energy which it transports; longer wavelength means that there is lesser energy, but the low frequency waves have wider T (period), while the high frequency waves have lower period, this can be viewed from the energy wave diagram below. A wave is an energy transport medium which transports energy along a medium without transporting matter. The amount of energy carried by a wave is related to the amplitude of the wave and directly proportional to the square of amplitude, this property has been used to generate the Spectrogram, which shows the amount of energy absorbed and contributed by each number in the pitch of the audio signal recorded.

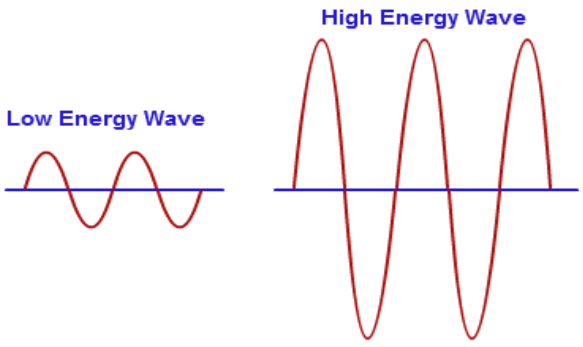


Figure 1: Wave Energy profile of Audio Signals

d) The Coding Procedure for the Algorithm

The speech recognition system algorithm is designed using a four layer neural network with four input neurons and a bias which is attached to each layer. The variable X_1 (size of the vocabulary) which is divided into small words i.e. 2-100words with weight of 0.70, medium words ranging from 100-1000 words with weight .25 and large words ranging from at least 10,000 words with weight 0.05. The un-forbidden code for recognising a small word is (100) the small words is coded with digit 1, while medium words and large words are coded with 0 respectively for this system to recognize the speech spoken in this research. The variable representing the second neuron is X_2 (Channel characteristics) is divided into low, medium and high with weights 0.05, .25 and 0.70 respectively for the neurons to recognize whether the channel is okay for the speech to be recognized. The three input neurons (x_{21}, x_{22}, x_{23}) which are the low channels characteristics, medium, and High vales of the input X_2 are chosen according to the prescribed weights to recognize and output value 1, with the patterns chosen as; 100, or 010, for suitability for speech recognition to be 1, for non-suitability, when the patterns are; 000 and 111 making it to be an XOR values. These required XOR output patterns which mark the threshold value, for recognized speech using the input neuron X_2. For the variable X_3 (the Speaking mode), his is divided into Isolated words, connected words, and continuous words are assigned with weights; 0.70, 0.25, and 0.05 with the suggested output digits; 100 and 110 is being regarded as high value 1 and the patterns 001, 111, being regarded as low value 0 or the forbidden codes for the neurons to recognize the speech spoken.

The above outcomes are from the three inputs neurons (x_{31}, x_{32}, x_{33}), which are the speaking mode values of the third input neurons. The forth variable X_4 (the types of noise), these are measured in terms of decibel values, the various divisions of the neurons are; less than 10Db, medium $10dB \leq X \leq 30dB$, and high values ranging $\geq 30dB$. The last bias is always assi9gned with digit value 1. The back-propagation algorithm ensures that the input data is repeatedly presented to the neural network in the training process. In each presentation the output of the neural network is compared to the desired output while the error is computed to see whether the neurons are actually predicting the speech. This error is then fed back to the neural network and is used to adjust the weights such that the error decreases with each cycle of the training and the neural model gets closer and closer to producing the desired output of the speech recognition.

The coding procedures as they are fed into the algorithm can be selected according to the following rules, $x_{11}^{x_1}, x_{21}^{x_2}, x_{31}^{x_3}, x_{41}^{x_4}, 1$ in the sequence one. It's worth noting that the last digit in all the cases is the bias, which is always digit 1. This is the way they have been supplied to the code in the python deep learning algorithm designed for this research.

e) Neural Architecture

The voice recognition system used in this research assumes the pattern of recurrent neural network, which conforms to the below architecture, but in actual sense of this research, four inputs have been used and the two separate hidden layers of the order of nine and six neurons in the middle preceding the output. They are many factors responsible for speech recognition of sound wave, but the most important four have been focused for the purpose of the research. The fifth neurons are the bias to make it a non-linear model, for easier recognitions speeches using the intelligent deep learning of neuron-computing. The processing neurons in the first and second hidden layers ensure that the threshold energy values in the spectrum are intelligently interpreted with accuracy in speed because they are tightly connected for faster information delivery to the output neurons.

For the purpose of this research, the training algorithm has been coded in python algorithmic language and the training was repeated with 250epoch to minimize the errors and getting a better output, which matched the threshold values in all the cases.

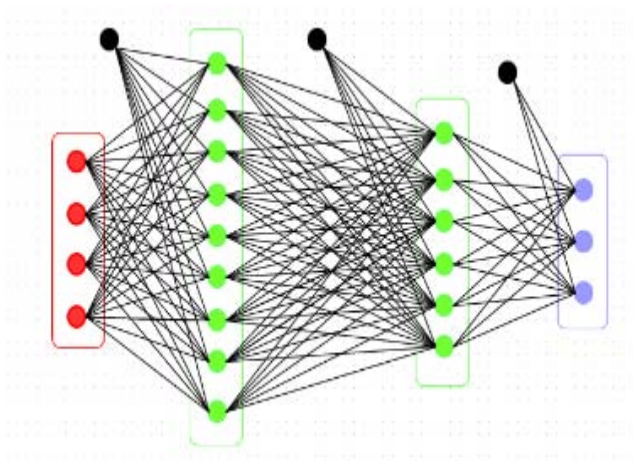


Figure 2: Network Architecture

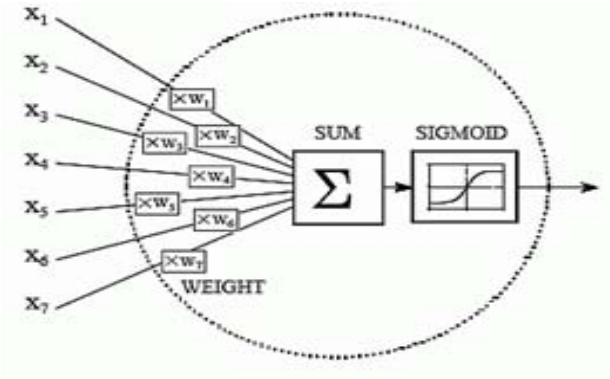


Figure 3: Neural Activation function

The Neural network model using the XOR data is repeatedly presented to the neural network.

At each presentation, the error between the network inputs, the hidden layers and the desired output were calculated, which is the threshold energy value when it has been activated through the sigmoid function. The computed values are then fed back to the neural network for proper adjustments. These sequences of events were done repeated until an acceptable error has been reached, when the network no longer appears to be learning, and the final output computed.

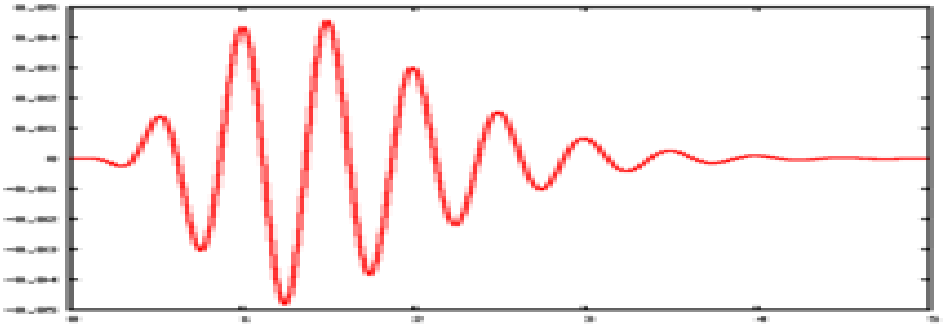
III. The Speech Recognition Principles

The following procedures were adopted for the speech recognition machine to fully act as an automatic speech recognizer; in other to fully develop an automatic speech recognition algorithm, the first step is to record an Audio signal from microphone, and store it in a file, thereafter sampling is carried out to select the portion of appreciable size, this is done using various sampling theorem, since sound waves are recorded as a continuous signals of varying amplitude, there is need to convert it into a discrete time signal in other make representation in digital form easier. The next step after this is to carry out the Fourier Transformation (FT) and Fast Fourier Transform (FFT), the extraction of the Audio signal is necessary in other to obtain the energy equivalent of the digitized signal which can be fed into neural Algorithm for deep learning to take and speech recognition to be achieved. These processes are discussed as a separate segment below.

a) The Sampling Method

Sampling can be defined as the acquisition of a continuous signal at a discreet time interval, since sound signal travel as waves an in one-dimensional plane. At every moment in time, they have a single value based on the height of the wave. For the purpose of this research a complex Audio signal of sampling size of 44,100Hz is assumed. The ideal sampling function $\delta_T(t)$ is a train of unit impulses defined as;

$\delta_T(t) = \sum_{n=-\infty}^{\infty} \delta(t - nT)$, where T is the sampling interval. A typical sound waves recorded can be viewed to have a complex structure like figure 1, but it involves thousands of wave forms, because of this, there is need to convert this to discreet time signal and convert it into numbers and bits to make easier for representation, this can be viewed in the figures 2 and 3 below. In this research, for speech recognition, a sampling rate of 16 kHz (16,000 samples per second) is enough to cover the frequency range of human speech in other to completely design an automatic speech recognition system.



Sampled segment of the Speech

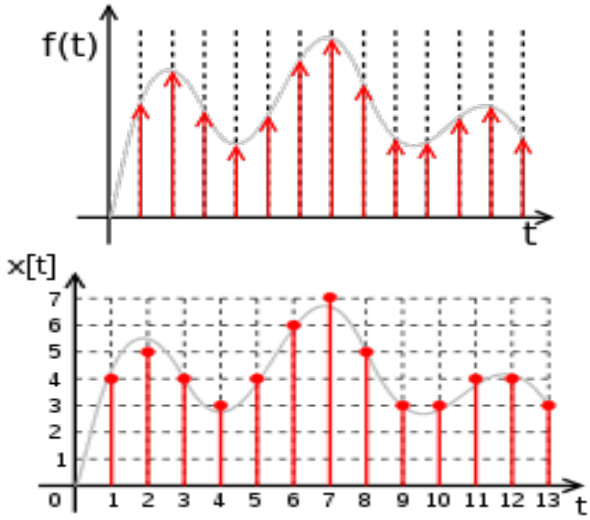


Figure 4: Sampled Audio Clip and Discreet sample

In other to turn this signal into numbers, there is need to record the maximum displacement at equally spaced points through the sampling process, which is shown in the figure 4.

By taking the a reading thousands of times a second and recording a number of the sound wave at that point in time, as in this research where a sampling size of 16000 samples per second enabled the machine to fully recognize the speech. To correct the errors in gaps, the research used NYQUIST theorem, which made it possible to perfectly reconstruct the original sound waves from the spaced out samples, as long as the Nyquist requirements are met; $w_s \geq 2w_{\max}$.

After the sampling, there is need to carry out some processing on Audio data by grouping the sampled Audio into 20 milliseconds long, this makes extraction easier on sample.

b) Characterisation of Audio Signals using Fourier Transform Techniques

The principles employed in this research involves converting the time domain signals into the frequency domain, and understanding its' frequency components using the mathematical tool of Fourier transform. This is important because it gives a lot of information about the sound signal in question.

This is the most powerful mathematical tool invented to characterise signals through transformation from time domain to frequency domain. The FFT has been used effectively by [4], [6] to recognise the voice of some physically challenged people who can only use their voices to register and attend examination. It was used to analyse spectrum to continuous signals where it was discovered that it was the faster mathematical method that eliminates redundancy in terms of signals which do not contain needed information. If given N sample size in time domain, and it is required to operate this in frequency domain; to convert each frame of N samples from time domain into frequency domain. The Fourier Transform is to convert the convolution of the glottal pulse U[n] and the vocal tract impulse response H[n] in the time domain. The mathematical representation of this statement can be expressed by the equation below:

$$Y(w) = FFT[h(t) * X(t)] - H(w) * X(w),$$

The mathematical complexities of this principles have been taken care of using commands in the python libraries of version 27X

If X (w), H (w) and Y (w) are the Fourier Transform of X (t), H (t) and
Y (t) respectively [2].

c) Extraction Method For The Audio Signals

This is the most useful tool when it comes to building a speech recognition system; it finds a useful application in converting our signals from the time domain to frequency domain. Since the signal must be converted into usable forms of features vector, which includes extraction techniques such as; MFCC, PLP, PLP-RASTA etc. The Mel Frequency Ceptral Coefficient is a powerful tool that has been used by many researchers to extract unique features of human voice. It is based on linear cosine transform of the log power spectrum on the non-linear Mel frequency scale, because of the equally spaced of the frequency band which make it possible to approximate human voice; it is useful in carrying out extraction of unique features[1], [3]. The expression $m = 2595\log_{10}(1+\frac{f}{100})$ is used to convert the normal frequency f to the Mel scale m. The advantage of the MFCC is that it relates to the energy absorbed in terms velocity and acceleration of the speech [2], [4].

The extraction process can be viewed as the means of separating the complex sound wave into its' components parts, since some of the notes are low pitched, next lower pitched and so on. The procedures of mathematical tool used are the efficacy of Fourier transform which breaks apart the complex sound wave into simpler forms making it up. By this method it is easier to measure the energy value of each pitch of frequency band.

It is not easy to recognise a complex sound wave by the neural network, but these difficulties can be overcome by breaking it down into components parts making it up in other to obtain the equivalent energy relating to the pitch of frequency band.

IV. Results And Discussion

a) Analysis of Visualizing the Audio Signal

The speech recognition analysis actually started from the recording of the Audio signal through a microphone as input the device; thereafter the recorded Audio signal is stored in a wave file. The processes of sampling commences as it has been described in the previous segment of this research, the python 2.7X was used to carry out the sampling at certain frequency and conversion into discreet form to obtain the numerical values using the following line of commands;

```
import numpy as np
import matplotlib.pyplot as plt
from scipy.io import wavfile
```

The above command lines read from the file while the path is provided by the using the command; *frequency_sampling, audio_signal = wavfile. read ("hello.wav"),* this will return two values that's the sampling frequency and the Audio values.

It is important to display the parameters like sampling frequency of the audio signal, data type of signal and its duration, by using the commands;

```
print('\nSignal shape:', audio_signal.shape)
print('Signal Datatype:', audio_signal.dtype)
print('Signal duration:', round(audio_signal.shape[0] /
float(frequency_sampling), 2), 'seconds'),
```

with these the normalisation of the signal can be done easily by invoking the command; *audio_signal = audio_signal / np.power(2, 15).* In this research for simplicity, the first 100 values were extracted to visualise the signal using the commands; *audio_signal = audio_signal [:100]*

```
time_axis = 1000 * np.arange(0, len(audio_signal), 1) /
float(frequency_sampling
plt.figure()
plt.plot(x_axis, signal_power, color='black')
plt.xlabel('Frequency (kHz)')
plt.ylabel('Signal power (dB)')
plt.show()
```

This can be seen in the figure5. This is the an output graph and data extracted for the above audio signal as shown in the image here

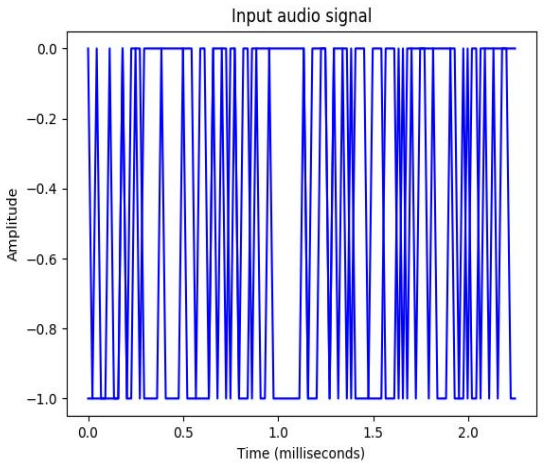


Figure 5: The Extracted Audio Signal

There is need to characterize these signals, characterizing an audio signal involves converting the time domain signal into frequency domain, and understanding its frequency components, by. This is an important step because it gives a lot of information about the signal. You can use a mathematical tool like Fourier Transform to perform this transformation. The processes of transformation using python 2.7X is achieved by invoking the following command lines;

```
import numpy as np
import matplotlib.pyplot as plt
from scipy.io import wavfile
from python_speech_features import mfcc, logfbank
```

frequency_sampling, audio_signal = wavfile. Read ("hello.wav")

print('\nSignal shape:', audio_signal.shape)

print('Signal Datatype:', audio_signal.dtype)

print('Signal duration:', round(audio_signal.shape[0] /

float(frequency_sampling), 2), 'seconds')

#normalization of audio

audio_signal = audio_signal / np.power(2, 15)

audio_signal = audio_signal [:100]

*time_axis = 1000 * np.arange(0, len(audio_signal), 1) / float (frequency_sampling*

The output of the transformation can be seen in the figure 6, in terms of the signal power on the frequency

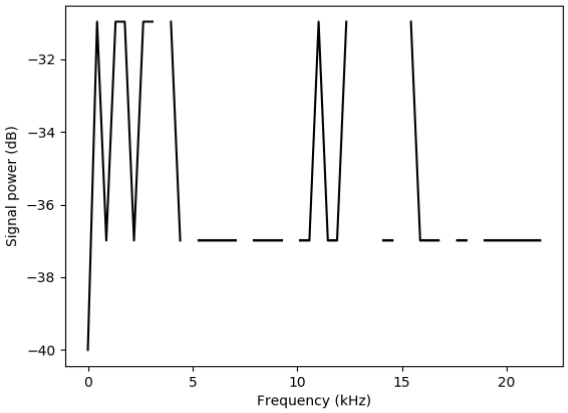


Figure 6: The Fourier Transformation Extraction

b) Features Extraction from Speech Analysis

This is the most important step in building a speech recognizer because after converting the speech signal into the frequency domain, the signals must convert it into the usable form of feature vector. We can use different feature extraction techniques like MFCC, PLP, and PLP-RASTA etc. for this purpose this research MFCC method has been adopted for the extraction using the following line of command;

import numpy as np

import matplotlib.pyplot as plt

from scipy.io import wavfile

from python_speech_features import mfcc, logfbank

frequency_sampling, audio_signal = wavfile. read ("hello.wav")

print('\nSignal shape:', audio_signal.shape)

print('Signal Datatype:', audio_signal.dtype)

print('Signal duration:', round(audio_signal.shape[0] /

float(frequency_sampling), 2), 'seconds')

#normalization of audio.

In other to display the MFCC values in terms of the energy absorbed by each frequency band in the spectrogram, there is need to invoke the following lines of command;

plt. matshow (filterbank_features)

plt. Title ('Filter bank')

plt. Show ()

This is displayed having two different platforms; Figure5 for MFCC and Figure 5a for Filter Bank.

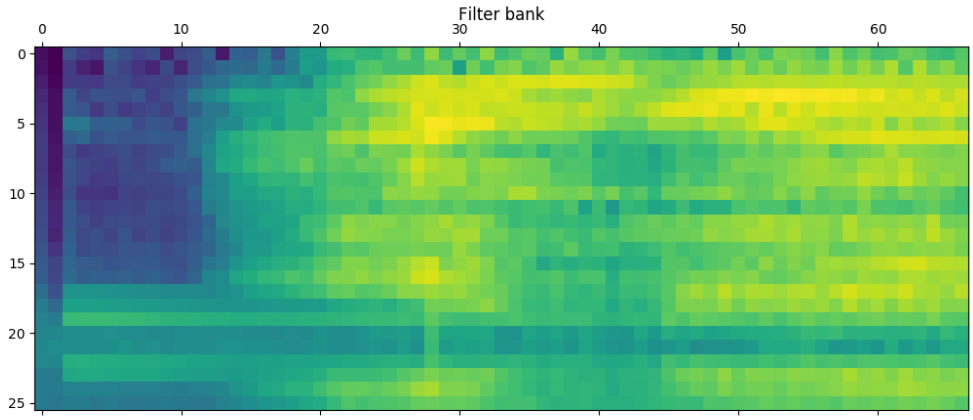


Figure 7: MFCC Extraction

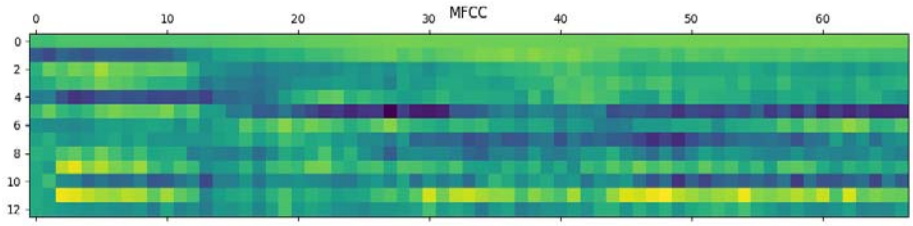


Figure 7a: The Filter Bank

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Fostering Residential Demand Response through Developing Proactive and Elastic Demand Approaches. An Overview DR

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Abstract- Demand response (DR) is one of the major stakeholders in the smart grid and has been used as an energy reconciler between supply and demand. After a literature overview, the importance of the paper is enhanced by having a theoretical and behavioral-based analysis of DR in power systems. In this work, the potential factors that influence more DR among customers and the residential market as a whole have been discussed. The customers' elastic demand approach can pave the way for adapting a responsive demand mechanism that ensures the system reliability and cost effective measures. Alternatively, this approach can make the program more effective and supportive in serving the social welfare as whole.

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Abstract- **Demand response (DR) is one of the major stakeholders in the smart grid and has been used as an energy reconciler between supply and demand. After a literature overview, the importance of the paper is enhanced by having a theoretical and behavioral-based analysis of DR in power systems. In this work, the potential factors that influence more DR among customers and the residential market as a whole, have been discussed. The customers' elastic demand approach can pave the way for adapting a responsive demand mechanism that ensures the system reliability and cost effective measures. Alternatively, this approach can make the program more effective and supportive in serving the social welfare as whole.**

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I. Introduction

The electricity management from production to transmission pose a permanent challenge for smart grid and power utilities. The increasing power demand with limited power amount puts pressure on power system, especially when it comes to widening peak-valley. With the development of information and communication technologies, demand side management (DSM) has become an important way improving the reliability of power systems by interacting both supply and demand [1]. The smart grid technology has made it possible to limit the customers' role in receiving the data and load rate through application of smart appliances at both demand and supply side. However, since DR provides an opportunity for the customers to regulate the real time grid conditions, the customers also deserve some of the benefits for their participation [2].The customers have two options in performing energy consumption, whether to participate voluntarily or for utility satisfaction. In this case, the volunteers forego their satisfaction over system reliability but the utility satisfaction will count when the total benefits, received by the customers, are more than comfort deviation (loss of satisfaction) due to peak reduction. The potential of DR further ensures the benefits for both entities (customers and suppliers) by focusing on consumption and supply pattern. Home energy management systems can play an important role in residential energy usage and home appliance technology coupled with rising populations. According to the World Business Council for Sustainable Development, approximately 40% of global energy consumption and 30% of carbon footprint are attributable to residential and commercial buildings [3]. This will likely lead to frequent blackouts and power curtailment during peak periods as well as rises in electricity prices.

The Demand Response (DR) is one of the potential solutions under smart energy management schemes that create a balanced manner between consumption and supply. According to the U.S. Department of Energy (DOE), demand response is a program established to incentivize the customers to change their normal consumption in response to changes in the electricity prices or when there is an emergency situation in the system [4]. The program further classifies into price-based DR (PBDR) and incentive-based DR (IBDR) [5]. In PBDR, customers reduce their normal consumption for price rise signals or emergency situations [6] [7]. The PBDR programs including real time (RTP) and time of use (TOU) energy pricing, which reduce power consumption during peak periods by utilizing peak and off-peak price differentials. IBDR refers to customers receiving financial benefits from reducing electricity consumption during the time, when the system experiences stress while providing additional power demand [4].

An important factor in the design of DR program understands how demand changes in response to incentives or tariff changes, which in economic terms is called the elasticity. Before the deregulation of the electricity network, elasticity was mainly used as a tool to understand customer load consumption and load forecast analysis [6]. In today's power market, elasticity is a powerful tool that is used to design demand response programs, especially for small customers.

DR programs that blend together customer education initiatives, enabling technology investments, dynamic pricing and customer behavior can achieve demand impacts that can alleviate the pressure on the power system. The objective of this paper is to foster the

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DR by active participation of demand side sources. As consumers become more aware of daily price fluctuations and respond through load curbing and shift to non-peak times (i.e. doing laundry at night). It has been witnessed in the literature that there are some cases where the immediate price signals and incentives are not available by communication infrastructure limitations. However, the rapid penetration of the smart metering systems has enabled real-time monitoring of the electricity consumption in the households. For instance, in Finland more than 80% of the households are equipped with smart metering technology capable of measuring the accumulated electricity consumption for each hour of the day. Thus, the dynamic pricing is technologically possible and such products are expected to appear to the market.

The potential of dynamic pricing has been discussed in [7] and customers prefer incentive-based DR to compensate financially against peak reduction. The customer elasticity of incentive-based DR has been discussed in the study [8] where the load is divided into two categories, flexible and non-flexible, in order to integrate the actual responsiveness of incentives. But the consumption patterns in response to price changes are entirely varying with time and scale. Here the paper needs to include the PBDR along with IBDR and is because end-user behavior needs two things, reward on peak saving and punishment on over consumption. The paper [9] has discussed about the distinction between IBDR and PBDR and used IBDR as a useful program that further prefer IBDR as customer friendly and motivated program but the general acceptance or rejection of program is always based on proactive behavior. It's because, customers are of two types; risk aversive and risk taker, the moment every individual behaves according to his/her possibility or time space. Similarly, in [10] suggest that people subject to punishment are more anxious and less satisfied to respond the PBDR and secondly people are more likely to accept the IBDR on their following peak shaving.

This paper focuses on ways and sources to foster residential DR by having a thorough study of related literature. In the current literature, there more has been discussed about the price and income elasticity and its estimation with consideration of DR but still such factors and sources that make DR more effective and successful among the residential customers have not been discussed thoroughly. In this work, a theoretical background has been driven and proposed a schematic modification of DR on the base of demand side management and some consumer behavioral capacities have been driven that play more potentially.

II. Overview Of DR At Household Level

Demand response (DR) refers to the responsiveness of the customer's normal consumption patterns in response to changes in the price of electricity over a specific time interval [11]. DR facilitates the reduction of power consumption and conserve the energy. In addition, it maximizes the capacity utilization of distribution system by reducing or eliminating the need to build new lines and power infrastructure. DR includes all intentional electricity consumption modifications by end-use customers that are intended to alter the timing, level of instantaneous demand, or total electricity consumption [12].

DR programs can roughly be classified into the following main categories according to the party that initiates the demand reduction action:

a) Price-Based Demand Response (PBDR)

The price based DR program depicts the actual cost for the electricity from production to the distribution in a system. In PBDR, consumers are granted time varying prices that are defined based on the electricity cost in different time periods [5]. The utilities are charged different prices according to end-user consumption behavior. The time-of-use scheme is split into two periods of peak and off-peak with high and low rates, respectively. The dynamic tariff rates motivate customers in reducing electricity consumption and shifting load from peak to off-peak in order to balance between supply and demand. The program further contains a real-time price (RTP) and time-of-use (TOU) scheme that reflect the marginal value of continuous electricity according to real-time power supply and the price charges on time. Prices are not predetermined but are subject to hourly changes.

Price-based (DR) can change the consumption pattern of the customers by price leverage in the power market. The analysis of the regular pattern between customer's power consumption and changing prices is important in the research of DR, which will affect the price setting in power market and the economic benefit of market bodies. Price elasticity of demand is a common measure used in economics to analyze the responsiveness of the quantity demanded of a good or service to a change in its price.

b) Incentive-Based Demand Response (IBDR)

Incentive-based (DR) schemes, incentive payments are paid to customers against the reduction of power when the system gets jeopardized or stressed [13]. In this program a set of demand reduction signals are issued by utility companies or the DR aggregators to the customers in the form of voluntary demand reduction requests or mandatory commands. Under the program utility providers can manage to supervise the demand side through direct controlling of the appliances or interrupting loads at certain space of time.

c) Communication-Based Demand Response (CBDR)

In this type of DR program smart technologies are commonly used in the residential areas and are connected with some local area networks (LAN) that

enable the utilities to receive and update the electricity consumption data from customer side. One of the most advanced communication tool is advanced metering infrastructure (AMI) that measure hourly usage data and signal further to the provider in real time [14]. There are certain cases in the residential sector that power bills often arrive at month's end with only an aggregate usage number, which makes tracking energy usage difficult for consumers. This is why, the lack of smart technology can create information vacuum between demand and supply that further affects more power outages and line losses in power system [15].

d) Rate-Based Demand Response (RBDR)

The rates are predetermined and charged dynamically based on various times of the day/week/year and the available reserve margin. Customers are informed before going to use and inserting appliances. The customers would pay the highest prices for peak hours and lowest prices for off-peak hours. The customer would respond voluntarily to the changes in the electricity prices.

e) Demand reduction bids

DR enables customers to manage the consumption pattern by scheduling appliances from peak to off-peak interval and share the saving amount of energy in trading market with demand aggregator. The bids would normally include the available demand reduction capacity and the price asked for. This program encourages mainly large customers to provide load reductions at prices that are convenient and adjustable [16].

f) Educating & trained customers

The installation of smart meters and technologies are not sufficient to make the customers educated about how and when to use these programs and take price response. For longer term, the market reforms and customer awareness about the pros and cons of DR program, customer interaction with smart applications will automatically make them alert in response at price increases. The communication infrastructure and smart meters are the essentials to facilitate about price response and demand response capabilities. Every user undertakes different measures under certain parameters, like economic benefits, utility satisfaction, less outages and system reliability. For making system reliable and efficient, customers need to be educated before implementing any pricing or technical policy in a power system. The general awareness among the end-users improve their knowledge about DR program and its acceptability at homes. This is the reason that households may perceive dynamic pricing as complex and not giving importance to personal preferences, because individual behavior shapes household consumption [17].

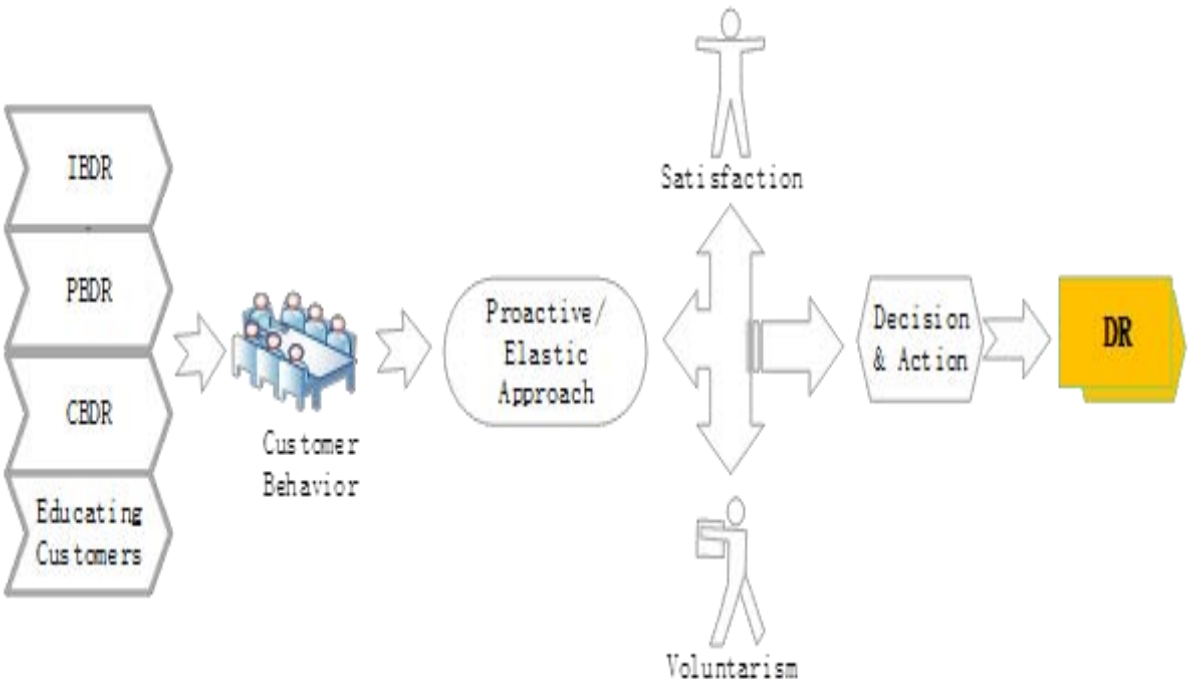

Figure 1: Proposed & schematic progression of DR in residential users.

III. Contribution And Future Implications

This study has been carried out with the underline scheme of residential demand behavior by considering a social welfare DR. In this work, focus is on consumers' preferences, motivations, benefits and system reliability under dynamic pricing mechanism. In Fig.1, effort has been made to capture the origin of DR from the beginning of household end-users. There are different types of DR programs that have been discussed in the literature, mainly referred as price-based demand response (PBDR) and incentive-based demand response (IBDR), respectively. Less focus has been put on measures and sources that instill the DR smoothly among the household end-users. The order and organization of factors motivating DR among the users have been highlighted that bring changes in consumption behavior of household. The study tried to capture different aspects linked to DR and likewise, the intrinsic link of DR with individual or social terms has also been discussed. More specifically, the purpose of this study is to obtain a wider understanding of the consumers preferences, and consumption behavior related to demand response with the following objectives, a) to draw a literature overview of DR program in respective of residential power scheduling; b) to educate each and every household understanding the DR by organizing conferences or door to door campaigns; c) to explore the factors that foster DR program among users and their motivation for taking part in DR; d) to obtain better understanding of parameters that could influence households' preferences between personal desires/satisfaction and voluntarism and being flexible in the electricity usage; and, e) at what extent DR contributes to the customers welfare.

This work can be improved by integrating social parameters along with customers' preferences for making DR a willing priority for every customer.

IV. Theoretical Background And Fostering the Program

Demand response programs that blend together customer education, enabling technology, and carefully designed dynamic rates can achieve demand impacts that can alleviate the system.

In this part of this paper, we thoroughly discuss and analyze the demand side factors that, by large, give an instrumental shift in consumer consumption pattern. We further, characterize our discussion of elastic demand, price and customer's elastic behavior approach in our next sections.

a) Definition and attributes of proactive and elastic steps in demand response

Despite the important role of elasticity in most kinds of DR designs, there are very few studies in the literature that shed a theoretical overview of DR. A thorough study is taken about the factors that promote and excel the DR program among the customers.

i. *Elasticity of demand*

An important factor in the design of demand response programs is understanding how demand changes in response to incentives or price changes, which in economic terms is called the elasticity. It was not so quick and smart communication, between end-user and utility, in the regulatory and traditional system [6]. In today's power market, elasticity is a powerful tool that can be used to design demand response programs, especially for small customers. In smart grid system, having use of DR programs, it is easy to check the customer's interaction level with utility prices through the demand elasticity. It has been discussed in both, IBDR and PBDR about the responsiveness of customers on following changes in price and given incentives. Both of programs, IBDR and PBDR, are recognized as simulators that instill the responsiveness or elasticity among the users on price signals [18][19].

ii. *Elastic and smart communication infrastructure*

The two-way communication enables customer to receive price signals at every level of time. In return, household individuals set their appliances by taking DR measures against changes in prices and incentives provided by utilities. The combination of dynamic prices with enablingtechnologies presents the most effective measure reducing the electricity consumption during peak hours [20]. With advanced metering infrastructure and communication, there are several benefits to aggregating the response of small residential loads; they can potentially provide more reliable response compared to a small number of large loads; the smaller residential loads may be able to provide a more continuous response than large loads [21].

Customers are equipped with smart meters and communication that can measure consumption at every interval of time and let customers know the price change. In most cases, residential customers have installed AMI by utility providers to take quick and countermeasure against price changes [22]. A recent study, customers are equipped with the device able to reduce their energy consumption by 6.5% compared to a statistically balanced control group that did not have the device.

iii. *Elastic consumption behavior and voluntarism*

In this part, the residential household reacts to the price changes with different level and quantity. If we talk about the DRM, there are numerous factors involved that influence customer's attitude towards a certain plan of action. But, somehow the economic factor has more effective involvement with consideration of dynamic prices and other financial incentives on consumption. In traditional power grids, customers are charged with

predetermined and predefined rates at each consumption period that result the customers remain reluctant while participating into smart grid operation. Usually, customer reluctance with DR is not by the customer consumption pattern or behavior but because of other factors like, customers living standard, demographical changes and by other alternative energy sources. The customer participating in the DR program generally categorize into two different levels; the customer taking risk is not usually sensitive or elastic on peak price changes but those who are active and have elastic behavior response the following changes and receiving incentives. Likewise, the customers who have knowledge about environment can have the power shifting passion to the green energy or off-peak time interval. Fig. 2 shows the different reactions of customers on elasticities. Consumer's response at dynamic pricing and other incentives is only possible by deregulated and technology installed market. [23]. However, it depends on consumer behavior that, sometimes, prefer energy conservation over individual satisfaction and willing to accept discomfort against given incentive or reward [24]. Sometimes, customers prefer social benefits over individual comfort and voluntarily participate in DR program.

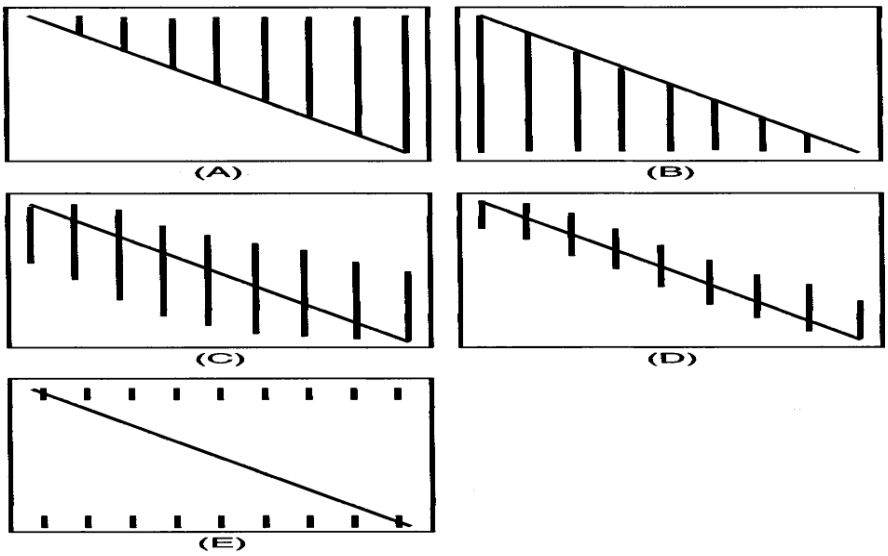

Figure 2: Customers consumption behavior at different price and time intervals. Adopted from (KIRSCHEN *et al*) [18].

iv. *Elastic financial rewards or penalties on consumption pattern*

The residential DR remains active as customers are convinced with greater availability of incentives to reduce peak demand that, as a result improve system reliability. It has been witnessed in [10] [25], that the customers subject to penalties are more anxious, less satisfied and less likely to respond, similarly on the other hand, customers are frankly to accept incentives than penalty of higher costs. More often, end-users maintain using the electricity until their marginal benefit is equal to the price paid. By using demand response management, that rely on dynamic pricing and incentives, as the main objective for altering electricity usage by shifting or directly control the load. Though, using prices to control demand is economically efficient as both the consumer and the utility benefits. It creates incentives for consumers to engage in energy conservation and efficiency and increases the options available to the utility provider to maintain security of the supply network [26]. Incentives and penalties have the equal and far lasting impact over consumption pattern, in the sense that small customers are usually risk averse and prefer incentives over penalties. Similarly, there are small customers that are risk taker and manage the consumption accordingly.

V. Fostering Dr and Social Contribution

Demand response program can be considered as a subset of customer consumption behavior and smart communication infrastructure that work together for the smart grid. The real time pricing signals and demand levels are transmitted through the smart communication and customers are notified with relevant penalties and incentives at the same time. Fig. 3 shows the measures that enhance the DR smoothly among residential households.

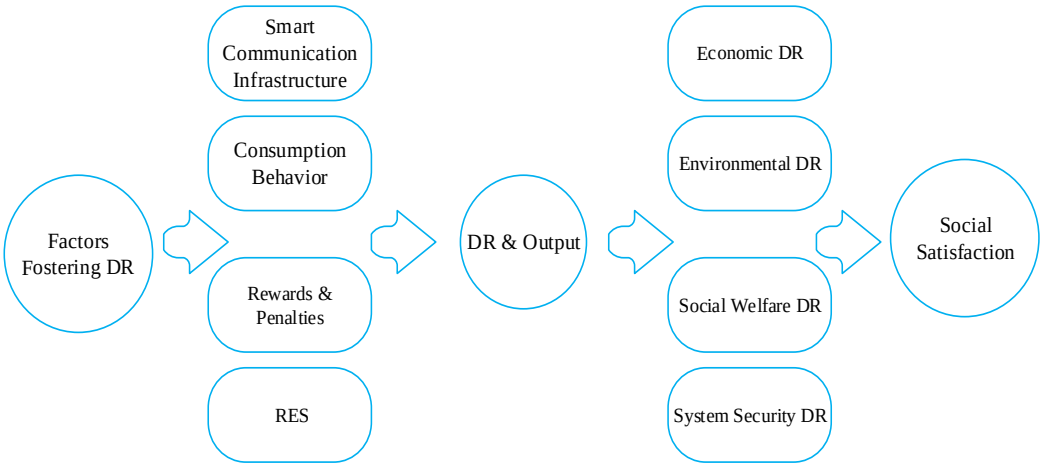

Figure 3: DR structure and social contribution.

a) Economic DR

The electricity consumption remains different among different customers, the reason is income elasticity of demand and general consumption behavior. In an elastic situation, customers actively participate in the demand response by acquiring financial and technical opportunities at home by suppliers [27]. End-use customers participate in these DR programs by using either distributed generators or energy management strategies to reduce the load in response to price signal from energy provider. The customers are notified about the varying prices by home displays at each interval of time to set the residential load economically and technically equal. For instance, the real-time price (RTP) and time-of use price (TOU) are the basic pricing mechanism that substantially create an economical DR environment among the customers. Economic DR participates in energy markets not only during emergencies but any time spot energy prices become high. This can make electricity markets more competitive and efficient by increasing the elasticity of demand. Allowing DR resources to compete against generating capacity also limits supplier market power. This can impact on mitigating peak prices and reducing price volatility [28].

The induction of DR into regulated and constrained electricity market can have potential for lowering the peak costs and have supervise over market power generators. Furthermore, it can increase the long run energy efficiency and system reliability by reducing peak and conserving energy. It has been witnessed in the literature that the monetary benefits are the sole motivation for users to participate in the program [29][30].

b) Environmental DR

Conventional power plants do not maintain the quantity demand and supply efficiently; when end-use customers demand increase, more power plants are constructed to meet the additional demand. Similarly, new technologies are used for generating power during peak time that, on the other hand, pose some harmful environmental impacts. The additional generation of electricity from fossil fuel in power plants releases several contaminants, such as SO2, NOx and CO2 into the atmosphere [31]. The demand side management empower the customer at making decisions that indirectly increases the system reliability, decreases cost and emission reduction and creating some revenue benefits the households.

There are two approaches to protect the environment. The use of emission free renewable energy and nuclear reactors is the first approach focusing on diversification of energy supply. The second is focusing on the demand side conservation of energy, by using energy efficient buildings and appliances. From generation perspectives, many energy policies have been initiated to encourage people to use renewable energy at micro level. Also there is encouragement to use large scale renewable energy mainly onshore and offshore wind turbines and photovoltaic farms.

c) Social welfare DR

Demand response (DR) refers to the dynamic demand mechanisms to manage customer consumption of electricity in response to supply conditions, in one of the most important function of smart grid [32]. In the smart grid, it is possible to realize the customer's active participation into demand side management (DSM) that further improve the functionality of DR among the households. The customer participatory DR is based on the combination of social welfare and system reliability, for instance, the maximization of the distributed generation consumption or the power limitation [33]. Similarly, the active DR in a household contains numerous advantages such as

reduction of electricity bills, peak load reductions and rationality with energy consumption. At result, customers have opportunity to bid the shaved load into the market when the prices exceed the customer's bid. As many incentives are offered in curtailment of power and organizing the appliances at peak intervals.

d) System reliability DR

Demand response (DR) program have been designed and developed for households' optimum satisfaction from utilization in power market. The program further motivates customers on peak shaving and valley filling in order to keep a balance between supply and demand in normal situation and in emergency time. It is associated with the short-term changes targeted for the critical hours when demand is high or reserve margin is low. In the short-term period, DR can improve the reliability of the power system and provide potential benefits for both the utility and the customers. On peak time, the program can reduce the power by scheduling the appliances from peak to off-peak and therefore postpone the construction and investments for the new power plants.

Previous studies have also identified the importance of induction of advance metering infrastructure (AMI) and building automation controls for enabling DR and energy efficiency [34]. In some cases, customers can not participate in these DR programs by using either distributed generators or energy management control strategies to reduce their load in response to a price or emergency signal utility [27]. However, the DR program connects users with smart and secure infrastructure to keep them up-to-date about consumptions, prices and the peak mode for grid safety.

e) Renewable energy sources (RES)

The smart grid has enabled the demand response as tool to adapt low electricity consumption pattern by customers from having low-electricity price during off-peak interval. Moreover, DR provides other potential advantages such as building self-electricity generators, lower volatilities in market prices, constructing renewable energy sources as alternative or stand-by generators and providing system reliability. The renewable sources have been preferred to adapt at emergency or peak hours to attain comfort level and reduce further demand at peak hours. In this context, 33% of the energy will be integrated from renewable energy sources in the United States by 2020 [35].

VI. Conclusions

The combination of advanced communication infrastructure and dynamic prices are considered the most effective program for reducing electricity demand during peak hours. Customers and utility providers are connected with smart meters by signaling price and demand updates at each time intervals. On the base of customer's consumption pattern, the utilities are entitled to set the price and incentives for reducing peak demand. Similarly, incentives and price-based demand response are used as tool for inducing customers on peak shaving and contributing system with renewable sources. But it depends on the consumer behavior whether to achieve the limited satisfaction or act voluntarily for social benefits (e.g., by selecting voluntarism or self-satisfaction options for longer purpose). For that, households need to go through a learning experience, activating the behavioral changes in interaction with the DR program, continuing the newly acquired behavior. Many different factors besides the prices, incentives and penalties, play an important role in this process: a) to educate each and every household about the importance of DR by organizing conferences or door to door campaigns; b) there is need to develop an elastic demand approach that could react to price changes by utilities. In order to make DR effective, elastic demand approaches through the application of information and communication technology (ICT), consumption pattern, rewards and penalties are recommended for residential customers. More research on elastic demand approach through empowerment of ICT, educating consumer and integrating demand side sources is thus needed.

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Vibrational Properties of Disorder Silicene

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Keywords: phonon density of state; defects; raman spectrum; lattice structure;brillouin zone.

I. Introduction

The field of nanomaterials has become one of the most quickly growing areas in science due to the unique properties and potential applications of these materials in electronics, medicine, consumer goods, defence, amongst others. Nanomaterials come in different shapes including zero-dimensional (0D), one-dimensional (1D) and two-dimensional (2D) forms. They are classified by having at least one of their dimensions less than 100 nm in size. The class of 2D nanomaterials are characterised by large lateral dimensions and small thicknesses of the order of less than, typically, several nanometres. They are often referred to as Nano sheets and can be considered akin to extremely thin sheets of paper. A wide variety of materials can be grown as 2D nanomaterials and can be composed of one or multiple elements. The elemental 2D nanomaterials usually have names ending in 'ene', namely silicene. Silicene is a crystalline two-dimensional (2D) nanomaterial composed entirely of silicon (Si) atoms. The atoms in this single layer are arranged in a hexagonal honeycomb structure which, when viewed from the side, are buckled [1].

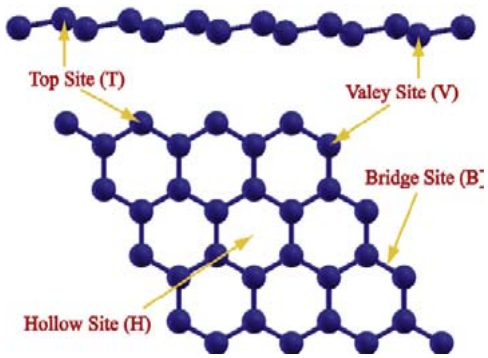

Figure 1: A (4 × 4) super cell of hexagonal buckled silicene structure

In fact, in view of the unique electronic properties found for the widest studied 2D material, graphene, researchers are looking for similar or even better properties in other layered materials, which could be eventually integrated into the current Nano electronics technology. Silicon is nowadays the most important semiconducting element used in this technology. Thus, the idea of having the silicon counterpart of graphene (silicene), is at the same time fascinating from the physical point of view, but also very attractive by virtue its possible integration into Nano electronics devices.

a) Objectives

We use force vibrational method for numerical analysis induced by Williams and Marris [121.s] and it is applicable for any disordered 2D material systems. We can apply this method as the field of

- A large complex disordered system.
- In low frequency regime we can calculate the DOS.

The main objectives of our thesis are:

- Develop a model based on FV method to determine vibrational properties of disordered silicene.
- To determine the Phonon Density of States (PDOS) of silicene.

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b) Geometrical Structure

Silicon is the most commonly used material in the semiconductor industry and is made of sp3-hybridized silicon (Si) atoms adopting the three dimensional diamond structure (figure 2.1(a)).

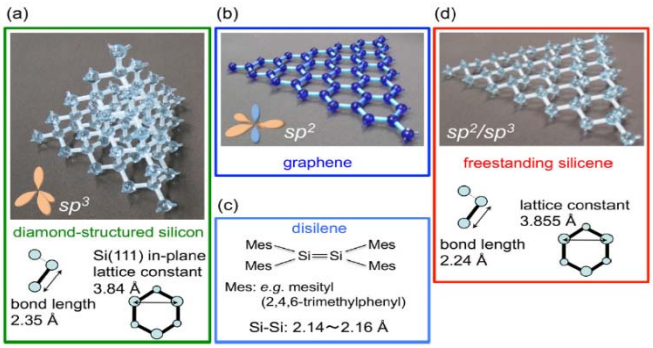

Figure 2: Structures and structural parameters of (a) diamond- structured silicon, (b) graphene (c) disilene [5], and (d) hypothetical, freestanding silicene [9]. In the insets, the sp^2 and sp^3 type of hybridization are sketch.

c) Lattice Structure

The lattice vectors of the hexagonal lattice with respect to the frame of reference used in the software Quantum Espresso are as follows: [16]

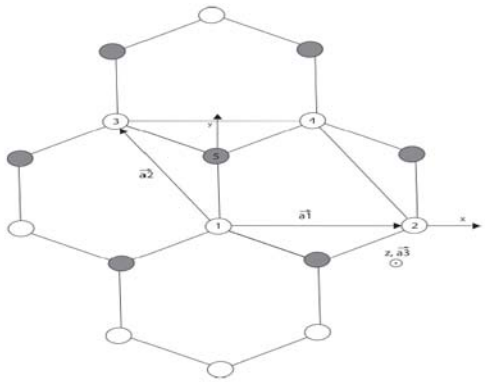

Figure 3: Lattice structure of silicene

$$\vec{a}_1 = a\hat{\imath}, \tag{1}$$

$$\vec{a}_2 = -\frac{a}{2}\hat{\imath} + \frac{\sqrt{3}a}{2}\hat{\jmath} \tag{2}$$

$$\vec{a}_3 = \hat{k} \tag{3}$$

The distance of this buckling parameter (Δz) is often given as 0.44 °A. [17] While silicene may seem three-dimensional due to the buckling parameter, it is more like a pseudo two-dimensional structure. The structure is actually two-dimensional except for that buckling parameter. Vector a_3 is only present for calculation reasons in the case of the two-dimensional structures. The buckling amount will be verified in the calculations section. Notice the buckling amount will vary when introduced into the bilayer and super lattice structure. But the buckling amount of stand-alone silicene will be verified so that Quantum Espresso can be proven effective.

d) Band Structure

Once the lattice structure is determined, the next step is to determine the band diagrams of these silicene-graphene composites. To accomplish that one needs to construct the Brillouin zone of this hexagonal lattice. The Brillouin zone has some symmetry points that will be used to plot the band structure. The equations for the reciprocal vectors as well as the equations for the points in the Brillouin zone used to plot the band structure are,

$$\vec{b}_1 = \frac{2\pi}{a\sqrt{3}}\left(\sqrt{3}\hat{k}x + \hat{k}y\right) \tag{4}$$

$$\vec{b}_2 = \frac{4\pi}{a\sqrt{3}}\hat{k}y \tag{5}$$

$$\vec{b}_3 = 2\pi\hat{k}z \tag{6}$$

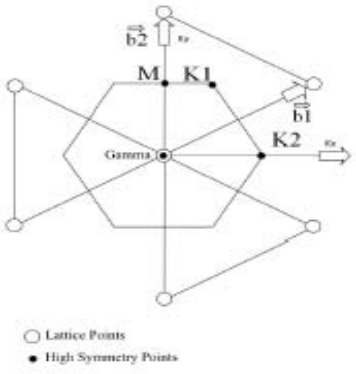

Figure 4: The Brillouin zone of silicene

The high symmetry points in the Brillouin zone will be written in this frame of reference. The units of $\frac{2\pi}{a}$ are pulled out to the front.Brillouin zone of the two materials will be the same.

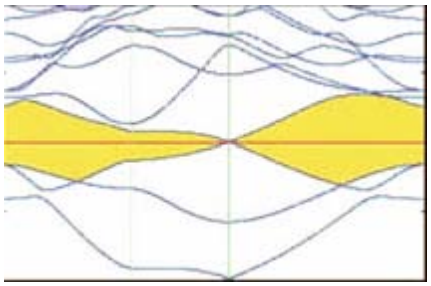

Figure 5: DFT band structure of silicene.

e) Phonons

Silicene has a flexural mode, as does graphene. However, because of the symmetry reduction due to the buckling, this mode for silicene has both a z and a xy component.

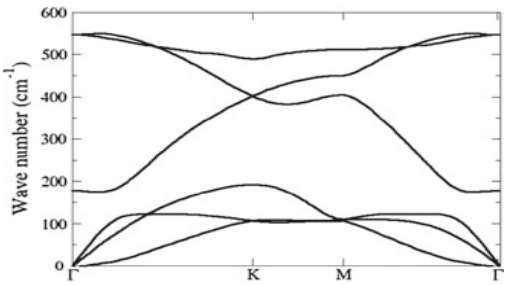

Figure 6: Phonon spectrum for silicene

f) Defects

When silicene-based materials have been fabricated experimentally, they will have some vacancy and atoms-vacancy defects [27]. Vacancies have a striking effect on the electronic structure. In particular, it is well known that vacancies induce localized states with associated resonant peaks at the Dirac point, and that state in the vicinity of the Dirac point has an enhanced tendency for localization, as revealed by an enhancement of the electronic inverse participation ratio [28].Variety of defects can exist in silicene and the impact on certain physical properties.

Single vacancies [33] and di-vacancies induce small gaps in silicene. Si atoms induce long-range spin polarization and a band gap, thus achieving an all-silicon magnetic semiconductor. Small defects were found to have a tendency to coalescence forming highly stable vacancy clusters [34].Stone-Wales defect is a topological defect formed by the 90° rotation of a dimer bond which results in four hexagons turning into two pairs of pentagon-heptagon rings.

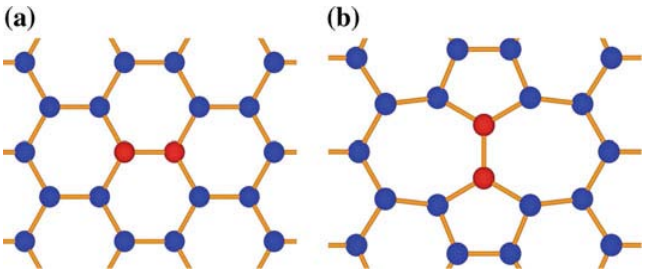

Figure 7: Representation of a stone-wales defect in silicene.

In particular, it was found that the formation energy and kinetic barrier are lower in silicene than in graphene. A band gap of 0.01 eV is created. The effect of vacancies and Stone-Wales defects on the mechanical properties has been studied using molecular dynamic finite element method with Turnoff potential [33]. They found that pristine and lowly defective silicene sheets exhibit almost the same elastic nature up to the fracture points. However, a single defect significantly weakened the silicene sheet, leading to a considerable reduction in the fracture strength. Thus, one 2-atom vacancy in the reduced the fracture stress by 1820 % and the fracture strain by 3335 %. The weakening effects of Stone-Wales defects varied with the tensile direction and the orientation of these defects.

A defect that is particular to 2D materials but absent for graphene is the buckling interface formed between two pieces of silicene with oppositely oriented buckling [34].This leads to a line defect that has a low formation energy but has a higher reactivity than the pristine silicene itself. The latter was deduced by studying the adsorption of a single gold atom and they turn out to have a binding energy of −3.50 eV.

II. Methodology

a) Numerical method

The equation of motion of the masses is

$$M_l \ddot{u}_l(t) = -\sum_{\acute{l}} \emptyset_{l\acute{l}} u_{\acute{l}}(t) \qquad (7)$$

Where, M_1 andu_l (t) are the mass and displacement of the l_th mass and ∅_ (ll´) describes the strength of the spring coupling atoms l and l´. The

displacement can be decomposed into a set of normal modes according to

$$u_l(t) = \sum_\lambda Q_\lambda(t) \frac{e_\lambda(t)}{\sqrt{M_l}}, \quad (8)$$

Where Q_λ is the amplitude of the normal mode λ and e_l (λ) is the displacement pattern or "polarization" vector of the mode λ. The {e_l (λ)} and the frequencies {ω_λ } satisfy the equations

$$\sum_{\acute{l}} \phi_{l\acute{l}} (M_l M_{\acute{l}})^{-\frac{1}{2}} e_{\acute{l}}(\lambda) = \omega_\lambda^2 e_l(\lambda) \quad (9)$$

Thus, to find the frequencies and displacement patterns of the normal modes one has to find the eigenvalues and eigenvectors of an N×N matrix. Conventional methods require a large amount of computer time as N becomes large. Thus, one has to find another approach.

b) Method for the Density of States

Start with each atom at rest and with zero displacement then apply a force on each atom given by $F_l \cos(\Omega t)$Where F_l is independent of time. After a time, large compared to the typical period of oscillation of the atoms, the total energy of the atom is,

$$E = \frac{1}{2}\sum_\lambda [\sum_l \frac{F_l e_l(\lambda)}{\sqrt{M_l}}]^2 \frac{\sin\{[(\omega_l - \Omega)/2]t\}^2}{(\omega_\lambda - \Omega)^2} \quad (10)$$

Thus, for large times the periodic force excites only those modes whose frequency is close to Ω.

$$F_l = F_0 \sqrt{M_l} \cos \Phi_l \quad (11)$$

Where F_0 is a constant and ϕ_l is a random quantity. If we average over all possible values of Φ_l we find that the average value of E is

$$\langle E \rangle = \frac{{F_0}^2}{4} \sum_\lambda \frac{\sin\{[(\omega_l - \Omega)/2]t\}^2}{(\omega_\lambda - \Omega)^2} \quad (12)$$

We have used the orthonormality of the mode patterns:

$$\sum_l e_l(\lambda) e_l(\acute{\lambda}) = \delta_{\lambda\acute{\lambda}} \quad (13)$$

The modes which contribute to the sum in equation 3.6 are those whose frequencies lie within about $\pm\left(\frac{2\pi}{t}\right)$ of Ω . Let us choose t such that

$$\Omega t \gg 1 , \quad (14)$$

$$\frac{4\pi N}{\omega_m t} \gg 1 \quad (15)$$

Where ω_m is the maximum frequency of the system. Equation (3.8) means that only modes in a narrow band of frequency on the scale of Ω contribution to the sum, equation (3.9) ensures that the number of such modes is much larger than unity. Thus, if there conditions are met we have

$$\langle E \rangle \approx \frac{\pi t {F_0}^2}{8} \sum_\lambda \delta(\omega_\lambda - \Omega) = \frac{\pi t {F_o}^2 N g(\Omega)}{8} \quad (16)$$

Where g(Ω) is the phonon density of states. Thus, provided that a way can be found to carry out the time development in the presence of the periodic force, we can find

$$g(\Omega) = \frac{8\langle E \rangle}{\pi t {F_o}^2} \quad (17)$$

For a sufficiently large system, one expects that it will not be necessary to carry out explicitly the average over all values of the make one random choice of the $\{\phi_l\}$.

c) Numerical Algorithm

The problem thus reduces to the solution of the equations of motion of the system in the presence of a periodic force. These equations can be written as,

$$\dot{v_l} = {M_l}^{-1}[\phi_{l\acute{l}} u_{\acute{l}}(t) + F_l \cos(\Omega t)] \quad (18)$$

$$\dot{u_l}(t) = v_l(t) \quad (19)$$

The standard approach to the time development is to replace t by nτ where τ is a small time step, and n an integer. Then a time development algorithm is

$$v_1(n+1) = v_l(n) + {M_l}^{-1}[\phi_{l\acute{l}} u_{\acute{l}}(t) + F_l \cos(\Omega t)]\tau \quad (20)$$

$$u_1(n+1) = u_n + v_l(n)\,\tau \quad (21)$$

Normally one would choose τ to be small scale of the system, i.e. the period τ_m of the highest frequency mode.

The initial set at t= 0 is prepared in which all atoms are at rest and have zero displacements. A random force is applied to each atom at rest, which is given by:

$$F_l \cos(\Omega t) = F_0 \sqrt{M_l} \cos(\phi l) \cos(\Omega t) \quad (22)$$

Where F_0 is a constant and ϕl varies from 0 to 2π. The corresponding equation of motion of the system becomes:

$$M_l \ddot{u}_l + \sum_{\acute{l}} \phi l \acute{l}\, u_{\acute{l}}(t) = F_0 \sqrt{M_l} \cos(\phi l) \cos(\Omega t) \quad (23)$$

The total energy of the system can be written as the summation of kinetic and potential energy as follows:

$$E(t) = K + U$$

$$= \frac{1}{2}\sum_l M_l \dot{u_l}^2(t) + \frac{1}{2}\sum_l \sum_{\acute{l}} u_l(t)\, \phi l \acute{l} u_{\acute{l}}(t)$$

$$= \frac{1}{2}(\sum_l M_l \dot{u_l}^2(t) + \sum_l \sum_{\acute{l}} u_l(t)\, \phi l \acute{l} u_{\acute{l}}(t)) \quad (24)$$

Thus, for large times the periodic external force excites only those modes whose frequency is close to. When average all possible values of ϕ_l and used the ortho-normality of the eigen-vector$\Omega e_l(\lambda)$, the average value of energy $\langle E \rangle$becomes,

$$\langle E \rangle = \frac{{F_0}^2}{4} \sum_\lambda \frac{\sin\{(\Omega - \omega_\lambda)/2^t\}^2}{(\Omega - \omega_\lambda)^2} \quad (25)$$

If we choose t such that

$$\frac{1}{\Omega} \ll t \ll \frac{4\pi N}{\omega_{max}} \quad (26)$$

Therefore, from Eq. 3.10, we can write:

$$\langle E(\Omega)\rangle = \frac{\pi t {F_0}^2}{8} \sum_\lambda \delta(\omega_\lambda - \Omega) \quad (27)$$

The density of states are related with the delta function by the following equation:

$$g(\Omega) = \frac{1}{N} \sum_\lambda \delta(\omega_\lambda - \Omega) \quad (28)$$

Therefore, we can write the density of the states of the system is

$$\langle E(\Omega)\rangle = \frac{\pi t {F_0}^2 N g(\Omega)}{8} \quad (29)$$

$$g(\Omega) = \frac{8\langle E(\Omega)\rangle}{\pi t {F_0}^2 N} \quad (30)$$

Thus, it could be obtained phonon density of states to carry out the time development in the presence of external force.

d) Raman Spectroscopy

Raman spectroscopy is a widely used experimental technique to identify the characteristic vibrational modes of materials. It is one of the most used optical techniques for the characterization of 2D materials like graphene. Several properties can be derived from the analysis of the Raman spectra, e.g., the shift in frequency of the Raman peaks has been successfully used to analysis flakes of layered materials such as 〖MoS〗_2and quantify the number of layers [40, 41]; similarly the Raman spectrum of graphene flakes has been used not only for the identification of the number of layers, but also to estimate the quality (in term of defects) of the graphene sheets [42, 43].

Note however that the splitting of the iTO and iLO at Γ could be due to an artifact of the DFT calculation and particularly to the slightly different bond length $a \neq b$ predicted by using the nonlinear core correction. Nevertheless, the iTO mode is very close to the LiO mode and its Raman spectra show only one peak at around 575 cm–1, as shown in Fig. 3.1 below.

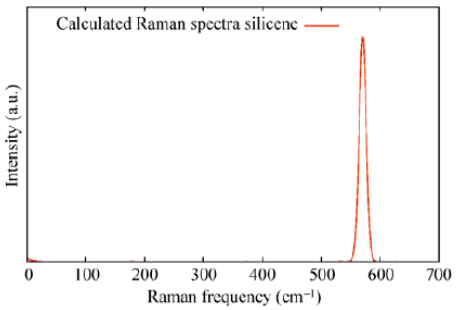

Figure 8: Raman spectrum of silicene obtained by the calculated vibrational spectrum convoluted with a uniform Gaussian broadening having 10 cm^{-1} width.

III. Result and Discussion

We have calculated phonon density of states of silicene, g(ω) for lattice of 1000 atoms in the array respectively 40×40 and we analysis for 5%,10% and 15% defects.We also have calculated phono density of states of silicene, g(ω) for lattice of 2000 atoms in the array respectively 50×50. We consider same 5%,10% and 15% defects for this lattice structure.

a) Force constants calculation

As the force constants are effective in three planes such that in the radius plane, in the inner plane, and in the outer plane. The force constants are as given following table 4.1[44].

Table 1: The force constants in three effective plane

Neighbour	Φ_{ra}	Φ_{tin}	Φ_{to}
1st	2.032544	15.9965	0.3814
2nd	-0.882486	0.9010	0.0683
3rd	0.249645	-0.9737	0.1396
4th	0.295442	-0.1067	0.1006

b) Results

Phonon Density of states of Silicene for different atom numbers:

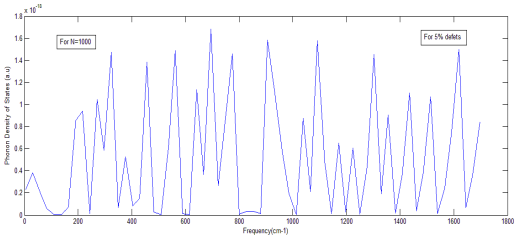

Figure 9: Phonon Density of States of silicene for 1000 atoms with 5% defects.

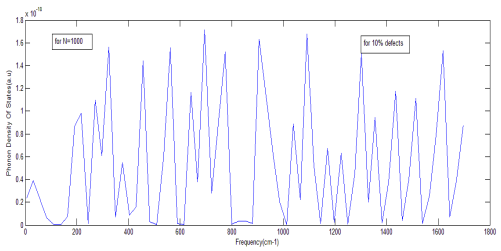

Figure 10: Phonon Density of States of silicene for 1000 atoms with 10% defects

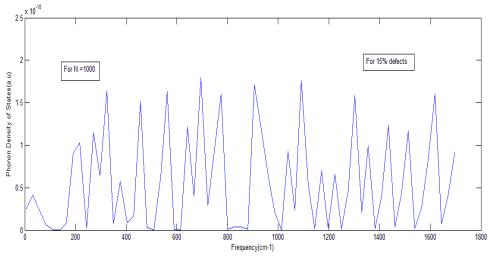

Figure 11: Phonon Density of States of silicene for 1000 atoms with 15% defects.

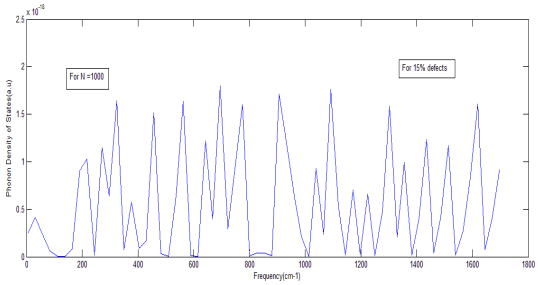

Figure 12: Phonon Density of States of silicene for 2000 atoms with 5% defets.

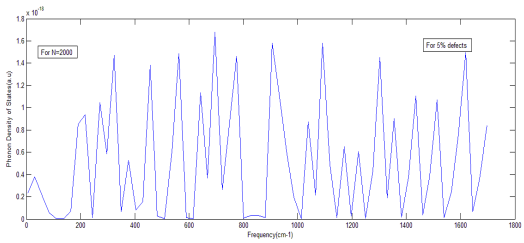

Figure 13: Phonon Density of States of silicene for 2007 atoms with 10% defects

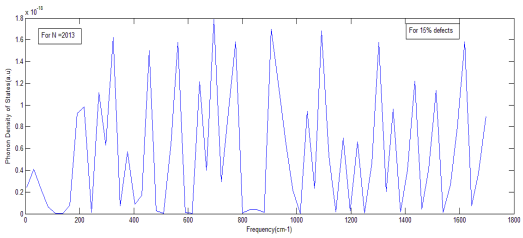

Figure 14: Phonon Density of States of silicene for 2013 atoms with 15% defects

IV. Conclusions and Future Work

Silicene is a single layer of silicon atoms with *sp3* bonds in the honeycomb lattice structure. More compatibility of the Silicene with the current semiconducting technology and some other advantages such as a new and promising alternative for the spintronic and the Nano-magnetic materials have attracted considerable scientific attention in very recent years. In addition, despite the single layer Graphene which owns zero band gap in the Dirac point, Silicene owns a tunable band gap from zero to semiconducting region, which make it better choice for the FET technology. However, stability of this material was an issue that the recent experimental studies showed that it could be stable with a small buckling. However, its electronic properties such as the density of states, the total carriers and the conductance as well as their temperature dependence and comparison with the electronic properties of the Graphene have been being investigating analytically.

We studied the Phonon Density of states (PDOSs) of disorder silicene, we belief that this thesis work will help to investigate the electronic properties of silicene. Of course, the work on silicene is still a growing area of research and there are many questions yet to be answered about the potential of this material. We are very excited to be part of the discoveries in this area and look forward to seeing where this material will go in the future. We hope that you as the reader will share in our passion for science and 2D nanomaterials!

The simulating analysis of vibrational properties like phonon density of states have been studied and found phonon density of states for lattice atoms disorder. There have been considered the normal mode of vibration. At the same time, there have been several important issues in the field that remain to be addressed.

We have performed the mathematical calculation on basis of a 2d dimensional model. The method developed in this dissertation can be extended to the three dimension for calculating the vibrational properties of multi-layer silicene. We can further calculate the layered structure of silicene and, further investigation of many-body interactions and electron-phonon scattering effect, calculation of Raman intensities, quantitative analysis of specific structural defects such as Stone-walse defects in silicene samples, and an harmonic effects responsible for the thermal conductivity in the silicene sheet. The electron-phonon interactions can be further calculated. The harmonic effects and thermal conductivity in the silicene sheet can be studied in a more systematic way.

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FELLOWS

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We shall provide you intimation regarding launching of e-version of journal of your stream time to time.This may be utilized in your library for the enrichment of knowledge of your students as well as it can also be helpful for the concerned faculty members.

The MARSE member can apply for approval, grading and certification of standards of their educational and Institutional Degrees to Open Association of Research, Society U.S.A.

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The Global Journals Incorporation (USA) at its discretion can also refer double blind peer reviewed paper at their end to the board for the verification and to get recommendation for final stage of acceptance of publication.

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The board can also take up the additional allied activities for betterment after our consultation.

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Note :

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- In future, if the board feels the necessity to change any board member, the same can be done with the consent of the chairperson along with anyone board member without our approval.
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- In case of "Difference of Opinion [if any]" among the Board members, our decision will be final and binding to everyone.

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Acknowledgments

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g) Suitable statistical data should also be given.
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20. Think technically: Always think technically. If anything happens, search for its reasons, benefits, and demerits. Think and then print: When you go to print your paper, check that tables are not split, headings are not detached from their descriptions, and page sequence is maintained.

21. Adding unnecessary information: Do not add unnecessary information like "I have used MS Excel to draw graphs." Irrelevant and inappropriate material is superfluous. Foreign terminology and phrases are not apropos. One should never take a broad view. Analogy is like feathers on a snake. Use words properly, regardless of how others use them. Remove quotations. Puns are for kids, not grunt readers. Never oversimplify: When adding material to your research paper, never go for oversimplification; this will definitely irritate the evaluator. Be specific. Never use rhythmic redundancies. Contractions shouldn't be used in a research paper. Comparisons are as terrible as clichés. Give up ampersands, abbreviations, and so on. Remove commas that are not necessary. Parenthetical words should be between brackets or commas. Understatement is always the best way to put forward earth-shaking thoughts. Give a detailed literary review.

22. Report concluded results: Use concluded results. From raw data, filter the results, and then conclude your studies based on measurements and observations taken. An appropriate number of decimal places should be used. Parenthetical remarks are prohibited here. Proofread carefully at the final stage. At the end, give an outline to your arguments. Spot perspectives of further study of the subject. Justify your conclusion at the bottom sufficiently, which will probably include examples.

23. Upon conclusion: Once you have concluded your research, the next most important step is to present your findings. Presentation is extremely important as it is the definite medium though which your research is going to be in print for the rest of the crowd. Care should be taken to categorize your thoughts well and present them in a logical and neat manner. A good quality research paper format is essential because it serves to highlight your research paper and bring to light all necessary aspects of your research.

Informal Guidelines of Research Paper Writing

Key points to remember:

- Submit all work in its final form.
- Write your paper in the form which is presented in the guidelines using the template.
- Please note the criteria peer reviewers will use for grading the final paper.

Final points:

One purpose of organizing a research paper is to let people interpret your efforts selectively. The journal requires the following sections, submitted in the order listed, with each section starting on a new page:

The introduction: This will be compiled from reference matter and reflect the design processes or outline of basis that directed you to make a study. As you carry out the process of study, the method and process section will be constructed like that. The results segment will show related statistics in nearly sequential order and direct reviewers to similar intellectual paths throughout the data that you gathered to carry out your study.

The discussion section:

This will provide understanding of the data and projections as to the implications of the results. The use of good quality references throughout the paper will give the effort trustworthiness by representing an alertness to prior workings.

Writing a research paper is not an easy job, no matter how trouble-free the actual research or concept. Practice, excellent preparation, and controlled record-keeping are the only means to make straightforward progression.

General style:

Specific editorial column necessities for compliance of a manuscript will always take over from directions in these general guidelines.

To make a paper clear: Adhere to recommended page limits.

Mistakes to avoid:

- Insertion of a title at the foot of a page with subsequent text on the next page.
- Separating a table, chart, or figure—confine each to a single page.
- Submitting a manuscript with pages out of sequence.
- In every section of your document, use standard writing style, including articles ("a" and "the").
- Keep paying attention to the topic of the paper.

- Use paragraphs to split each significant point (excluding the abstract).
- Align the primary line of each section.
- Present your points in sound order.
- Use present tense to report well-accepted matters.
- Use past tense to describe specific results.
- Do not use familiar wording; don't address the reviewer directly. Don't use slang or superlatives.
- Avoid use of extra pictures—include only those figures essential to presenting results.

Title page:

Choose a revealing title. It should be short and include the name(s) and address(es) of all authors. It should not have acronyms or abbreviations or exceed two printed lines.

Abstract: This summary should be two hundred words or less. It should clearly and briefly explain the key findings reported in the manuscript and must have precise statistics. It should not have acronyms or abbreviations. It should be logical in itself. Do not cite references at this point.

An abstract is a brief, distinct paragraph summary of finished work or work in development. In a minute or less, a reviewer can be taught the foundation behind the study, common approaches to the problem, relevant results, and significant conclusions or new questions.

Write your summary when your paper is completed because how can you write the summary of anything which is not yet written? Wealth of terminology is very essential in abstract. Use comprehensive sentences, and do not sacrifice readability for brevity; you can maintain it succinctly by phrasing sentences so that they provide more than a lone rationale. The author can at this moment go straight to shortening the outcome. Sum up the study with the subsequent elements in any summary. Try to limit the initial two items to no more than one line each.

Reason for writing the article—theory, overall issue, purpose.

- Fundamental goal.
- To-the-point depiction of the research.
- Consequences, including definite statistics—if the consequences are quantitative in nature, account for this; results of any numerical analysis should be reported. Significant conclusions or questions that emerge from the research.

Approach:

- Single section and succinct.
- An outline of the job done is always written in past tense.
- Concentrate on shortening results—limit background information to a verdict or two.
- Exact spelling, clarity of sentences and phrases, and appropriate reporting of quantities (proper units, important statistics) are just as significant in an abstract as they are anywhere else.

Introduction:

The introduction should "introduce" the manuscript. The reviewer should be presented with sufficient background information to be capable of comprehending and calculating the purpose of your study without having to refer to other works. The basis for the study should be offered. Give the most important references, but avoid making a comprehensive appraisal of the topic. Describe the problem visibly. If the problem is not acknowledged in a logical, reasonable way, the reviewer will give no attention to your results. Speak in common terms about techniques used to explain the problem, if needed, but do not present any particulars about the protocols here.

The following approach can create a valuable beginning:

- Explain the value (significance) of the study.
- Defend the model—why did you employ this particular system or method? What is its compensation? Remark upon its appropriateness from an abstract point of view as well as pointing out sensible reasons for using it.
- Present a justification. State your particular theory(-ies) or aim(s), and describe the logic that led you to choose them.
- Briefly explain the study's tentative purpose and how it meets the declared objectives.

Approach:

Use past tense except for when referring to recognized facts. After all, the manuscript will be submitted after the entire job is done. Sort out your thoughts; manufacture one key point for every section. If you make the four points listed above, you will need at least four paragraphs. Present surrounding information only when it is necessary to support a situation. The reviewer does not desire to read everything you know about a topic. Shape the theory specifically—do not take a broad view.

As always, give awareness to spelling, simplicity, and correctness of sentences and phrases.

Procedures (methods and materials):

This part is supposed to be the easiest to carve if you have good skills. A soundly written procedures segment allows a capable scientist to replicate your results. Present precise information about your supplies. The suppliers and clarity of reagents can be helpful bits of information. Present methods in sequential order, but linked methodologies can be grouped as a segment. Be concise when relating the protocols. Attempt to give the least amount of information that would permit another capable scientist to replicate your outcome, but be cautious that vital information is integrated. The use of subheadings is suggested and ought to be synchronized with the results section.

When a technique is used that has been well-described in another section, mention the specific item describing the way, but draw the basic principle while stating the situation. The purpose is to show all particular resources and broad procedures so that another person may use some or all of the methods in one more study or referee the scientific value of your work. It is not to be a step-by-step report of the whole thing you did, nor is a methods section a set of orders.

Materials:

Materials may be reported in part of a section or else they may be recognized along with your measures.

Methods:

- Report the method and not the particulars of each process that engaged the same methodology.
- Describe the method entirely.
- To be succinct, present methods under headings dedicated to specific dealings or groups of measures.
- Simplify—detail how procedures were completed, not how they were performed on a particular day.
- If well-known procedures were used, account for the procedure by name, possibly with a reference, and that's all.

Approach:

It is embarrassing to use vigorous voice when documenting methods without using first person, which would focus the reviewer's interest on the researcher rather than the job. As a result, when writing up the methods, most authors use third person passive voice.

Use standard style in this and every other part of the paper—avoid familiar lists, and use full sentences.

What to keep away from:

- Resources and methods are not a set of information.
- Skip all descriptive information and surroundings—save it for the argument.
- Leave out information that is immaterial to a third party.

Results:

The principle of a results segment is to present and demonstrate your conclusion. Create this part as entirely objective details of the outcome, and save all understanding for the discussion.

The page length of this segment is set by the sum and types of data to be reported. Use statistics and tables, if suitable, to present consequences most efficiently.

You must clearly differentiate material which would usually be incorporated in a study editorial from any unprocessed data or additional appendix matter that would not be available. In fact, such matters should not be submitted at all except if requested by the instructor.

Content:

- Sum up your conclusions in text and demonstrate them, if suitable, with figures and tables.
- In the manuscript, explain each of your consequences, and point the reader to remarks that are most appropriate.
- Present a background, such as by describing the question that was addressed by creation of an exacting study.
- Explain results of control experiments and give remarks that are not accessible in a prescribed figure or table, if appropriate.
- Examine your data, then prepare the analyzed (transformed) data in the form of a figure (graph), table, or manuscript.

What to stay away from:

- Do not discuss or infer your outcome, report surrounding information, or try to explain anything.
- Do not include raw data or intermediate calculations in a research manuscript.
- Do not present similar data more than once.
- A manuscript should complement any figures or tables, not duplicate information.
- Never confuse figures with tables—there is a difference.

Approach:

As always, use past tense when you submit your results, and put the whole thing in a reasonable order.

Put figures and tables, appropriately numbered, in order at the end of the report.

If you desire, you may place your figures and tables properly within the text of your results section.

Figures and tables:

If you put figures and tables at the end of some details, make certain that they are visibly distinguished from any attached appendix materials, such as raw facts. Whatever the position, each table must be titled, numbered one after the other, and include a heading. All figures and tables must be divided from the text.

Discussion:

The discussion is expected to be the trickiest segment to write. A lot of papers submitted to the journal are discarded based on problems with the discussion. There is no rule for how long an argument should be.

Position your understanding of the outcome visibly to lead the reviewer through your conclusions, and then finish the paper with a summing up of the implications of the study. The purpose here is to offer an understanding of your results and support all of your conclusions, using facts from your research and generally accepted information, if suitable. The implication of results should be fully described.

Infer your data in the conversation in suitable depth. This means that when you clarify an observable fact, you must explain mechanisms that may account for the observation. If your results vary from your prospect, make clear why that may have happened. If your results agree, then explain the theory that the proof supported. It is never suitable to just state that the data approved the prospect, and let it drop at that. Make a decision as to whether each premise is supported or discarded or if you cannot make a conclusion with assurance. Do not just dismiss a study or part of a study as "uncertain."

Research papers are not acknowledged if the work is imperfect. Draw what conclusions you can based upon the results that you have, and take care of the study as a finished work.

- You may propose future guidelines, such as how an experiment might be personalized to accomplish a new idea.
- Give details of all of your remarks as much as possible, focusing on mechanisms.
- Make a decision as to whether the tentative design sufficiently addressed the theory and whether or not it was correctly restricted. Try to present substitute explanations if they are sensible alternatives.
- One piece of research will not counter an overall question, so maintain the large picture in mind. Where do you go next? The best studies unlock new avenues of study. What questions remain?
- Recommendations for detailed papers will offer supplementary suggestions.

Approach:

When you refer to information, differentiate data generated by your own studies from other available information. Present work done by specific persons (including you) in past tense.

Describe generally acknowledged facts and main beliefs in present tense.

The Administration Rules

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Please note that following table is only a Grading of "Paper Compilation" and not on "Performed/Stated Research" whose grading solely depends on Individual Assigned Peer Reviewer and Editorial Board Member. These can be available only on request and after decision of Paper. This report will be the property of Global Journals.

Topics	Grades		
	A-B	**C-D**	**E-F**
Abstract	Clear and concise with appropriate content, Correct format. 200 words or below	Unclear summary and no specific data, Incorrect form Above 200 words	No specific data with ambiguous information Above 250 words
Introduction	Containing all background details with clear goal and appropriate details, flow specification, no grammar and spelling mistake, well organized sentence and paragraph, reference cited	Unclear and confusing data, appropriate format, grammar and spelling errors with unorganized matter	Out of place depth and content, hazy format
Methods and Procedures	Clear and to the point with well arranged paragraph, precision and accuracy of facts and figures, well organized subheads	Difficult to comprehend with embarrassed text, too much explanation but completed	Incorrect and unorganized structure with hazy meaning
Result	Well organized, Clear and specific, Correct units with precision, correct data, well structuring of paragraph, no grammar and spelling mistake	Complete and embarrassed text, difficult to comprehend	Irregular format with wrong facts and figures
Discussion	Well organized, meaningful specification, sound conclusion, logical and concise explanation, highly structured paragraph reference cited	Wordy, unclear conclusion, spurious	Conclusion is not cited, unorganized, difficult to comprehend
References	Complete and correct format, well organized	Beside the point, Incomplete	Wrong format and structuring

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