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Research Article

Study On Tharmal And Thermoelectric Properties Of Tin Selenied (Snse) And Quantum Well Structure

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Abstract

Tin selenide has attracted much attention in the thermoelectric community. Computational method is a that method that uses principle of computer science to assist in solving problem. It uses the result of theoretical approach incorporated into efficient computer program, to calculate the structure and properties of molecule and solid. In practical use, it is various scientific disciplines. Computational Science allows building models that allow making prediction of what might happened in the lab. So that perhaps better prepared to make good or to understand experiments that might be too expensive or too dangerous to do the lab, although computational method cannot replace the real laboratory work, it may become a vital tool for the exploration of scientific knowledge.

In present project work, we study how spatial confinement of acoustic phonon modes changes the thermoelectric figure of merit of quantum well structur via modification of the lattice thermal condutivity.

INTRODUCTON

COMPUTATIONAL MATERIAL SCIENCE:

I. INTRODUCTION:-

Computational method is a that method that uses principle of computer science to assist in solving problume.it uses the result of theoretical approach incorporated into efficient computer program, to calculated the structure and properties of molecule and solid. in practical use, it is various scientific disciplines

Research develop computer program, application software that modal system being studied and run these program with various sets of input parameter.typical,these model require massive amount of calculation (usually floating-point) and are often executed on supercomputer or distributed computing platforms numerical analysis is an important techniques used in computation science research can be categorized in three broad areas which are classified as computational science, experimental science and theatrical science.

Computational science is application of and numerical technique to solve large amd complex problem. Computational science takes advantage of not only the improvements in computer hardware, but probably more impotent the increments in computer algorithms and mathematical techniques. Computational science allow doing the things that were previously too difficult to do due to the complexity of the mathematics, the large number of calculation involved of combination of the two. Computational Science allows building models that allow making prediction of what might happened in the lab. So that perhaps better prepared to make good or to understand experiments that might be too expensive or too dangerous to do the lab, although computational method cannot replace the real laboratory work, it may become a vital tool for the exploration of scientific knowledge.

The definition of the computer science can be written as an interdisciplinary approach to the solution of complex problems. That uses concept and skills form the discipline of science, and mathematics

The main advantage of computational science is that it is fairly economical and eco-friendaly.it can model and stimulate the scientific problem accurately: therefore it is becoming more and more reliable tool for describe the experiment outcome.

TIN SELENIED (SnSe)

CRYSTAL STRUCTURE AND COPUTATIONAL METHOD

CRYSTAL STRUCTURE OF SnSe

Tin selenide, also known as stannous selenide, is an inorganic compound with the formula (SnSe), where Tin has a +2 oxidation state. Tin(II) selenide is a narrow band-gap (IV-VI) semiconductor and has received considerable interest for applications including low-cost photovoltaic and memory-switching devices.[2] Tin(II) Selenied is a typical layered metal chalcogenide;[3] that is, it includes a Group 16 anion (Se^{2-}) and an electropositive element (Sn^{2+}), and it is arranged in a layered structure.

Tin(II) selenide exhibits low thermal conductivity as well as reasonable electrical conductivity, creating the possibility of it being used in thermoelectric materials.[4] In 2014, a team at Northwestern University has established the world record performance for thermoelectric material efficiency

Tin selenide films have great potential in photovoltaic systems [1] as well as their applications as memory switching devices. Because of their anisotropic character, the tin chalcogenides are attractive layered compounds, and can be used as cathode materials in lithium intercalation batteries [2]. The indirect character of the bandgap of SnSe (B0.9 eV) is a common property of orthorhombic IV–VI compounds [3,4] and has been confirmed by band structure calculations for

Structure

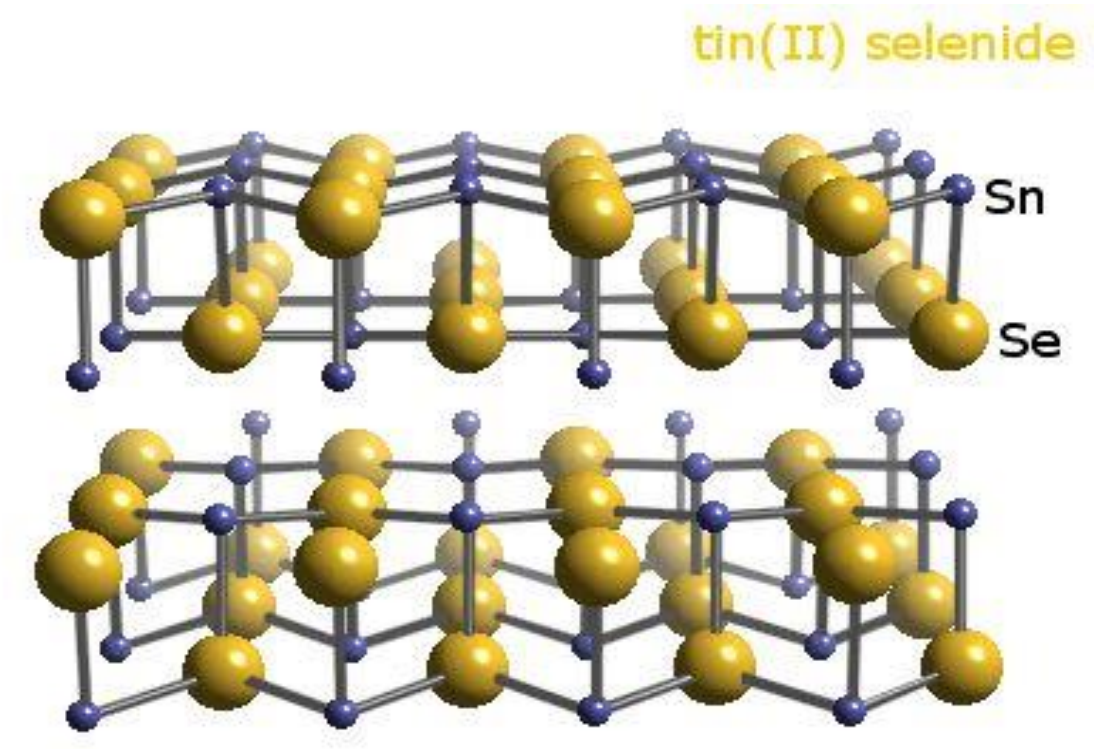
Tin (II) selenide can be formed by reacting the elements tin and selenium above 350 °C.

Problems with the composition are encountered during synthesis. Two phases exist—the hexagonal $SnSe_2$ phase and the orthorhombic SnSe phase. Specific nanostructures can be synthesized, but few 2D nanostructures have been prepared. Both square SnSe nanostructures and single-layer SnSe nanostructures have been prepared. Historically, phase-controlled synthesis of 2D tin selenide nanostructures is quite difficult.[3]

Sheet-like nanocrystalline SnSe with an orthorhombic phase has been prepared with good purity and crystallization via a reaction between a selenium alkaline aqueous solution and tin (II) complex at room temperature under atmospheric pressure.[11] SnSe Nano crystals have also been synthesized by a gas-phase laser photolysis reaction that used $Sn(CH_3)_4$ and $Se(CH_3)_2$ as precursors.

Crystalline 2×2-atom SnSe nanowire inside a single-wall carbon nanotube (tube diameter ~1 nm)[1]

A few-atom-thick SnSe nanowires can be grown inside narrow (~1 nm diameter) single-wall carbon nanotubes by heating the nanotubes with SnSe powder in vacuum at 960 °C. Contrary to the bulk SnSe, they have the cubic crystal structure



PROPERTRY OF SnSe is

Chemical formula	SnSe
Molar mass	197.67 g/mol
Appearance	steel gray odorless powder
Density	6.179 g/cm^3
Melting point	861 °C (1,582 °F; 1,134 K)
Solubility in water	nsoluble
Band gap	0.9 eV (indirect), 1.3 eV (direct)

Software used: Origin 8.0; MATLAB:

i) ORIGIN 8.0:

Origin is a proprietary program interactive scientific graphing and data analysis is produced by origin Lab Corporation, and run on Microsoft Windows. Graphing support in origin includes various 2D/3D oblique field plot types. Data analysis in origin imports Data files in various formats such as AFCITEXT,EXEL,NI-TDN,BID MEM NetCDF,SPC,CTC It also export the graph to various image files format such as JPEG,GIF,PPS,TIFF etc.

In origin the graph in Window is a container graphical depiction of experiment data and analysis result. Graph Window may contain a single plot in single graph layers. The graph layer is fundamental unit of the origin graph. The layer is comprises of bright of a set of axis scale values, one or more data plots, and any include text object etc. Graph layer can be created, size, and moved independently of one another.

ii)MATLAB:

MATLAB is the material science lab.MATLAB through characterized curve of the material studio is a flexible clean server software environment that brings some of the world most advanced material simulation and modeling technology to the PC.

Material studio makes it easy to create and study modals of molecular structures, exploiting stunninggraphics capabilities to presents the result. Integration with standard PC productivity tools facilities communication of these data. Material studies in visuals, which make is easy for to construct and manipulate graphic modal of molecules, organic and inorganic crystal. Polymer, amorphous materials, surface and layeredstructure.

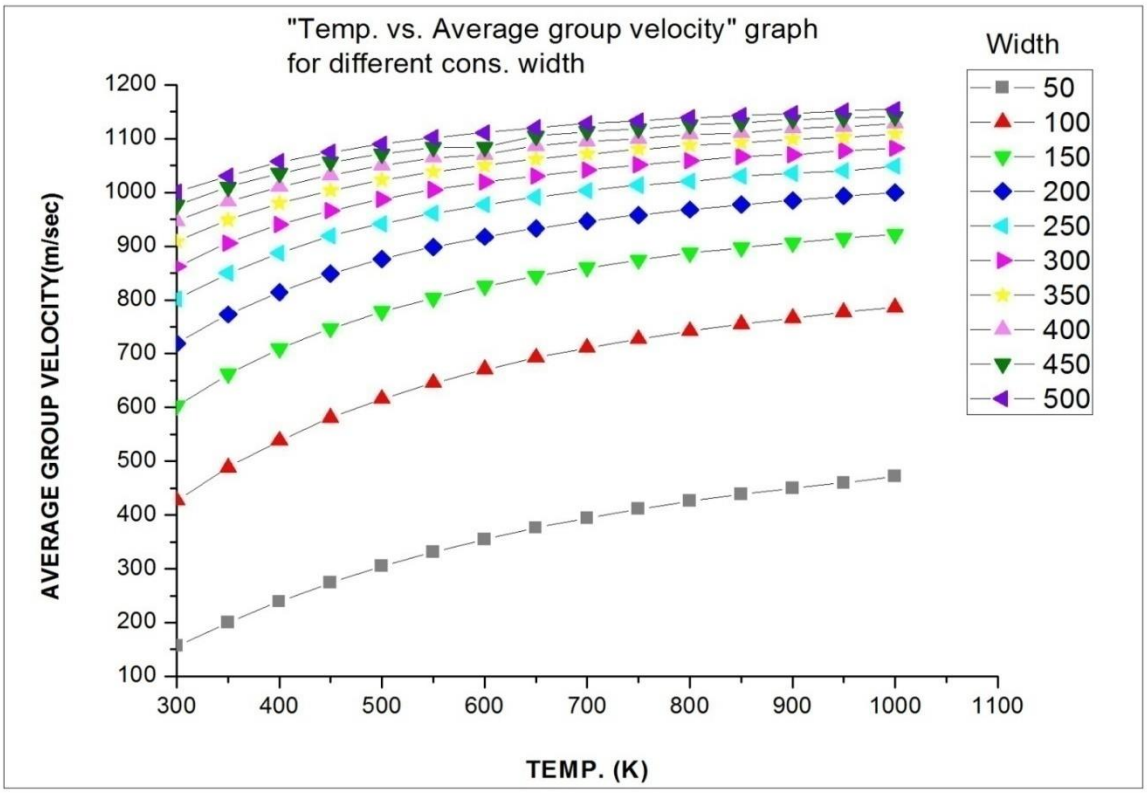
Material studios 6.1 include range of productivity improvements and new functionality that further extend application in topical are of research such as new functional material of energy applications.

RESULT AND DISCUSSION

THARMAL PROPERTIES OF SnSe:

Average group velocity (v_c):

i) The variation of average group velocity with temperature

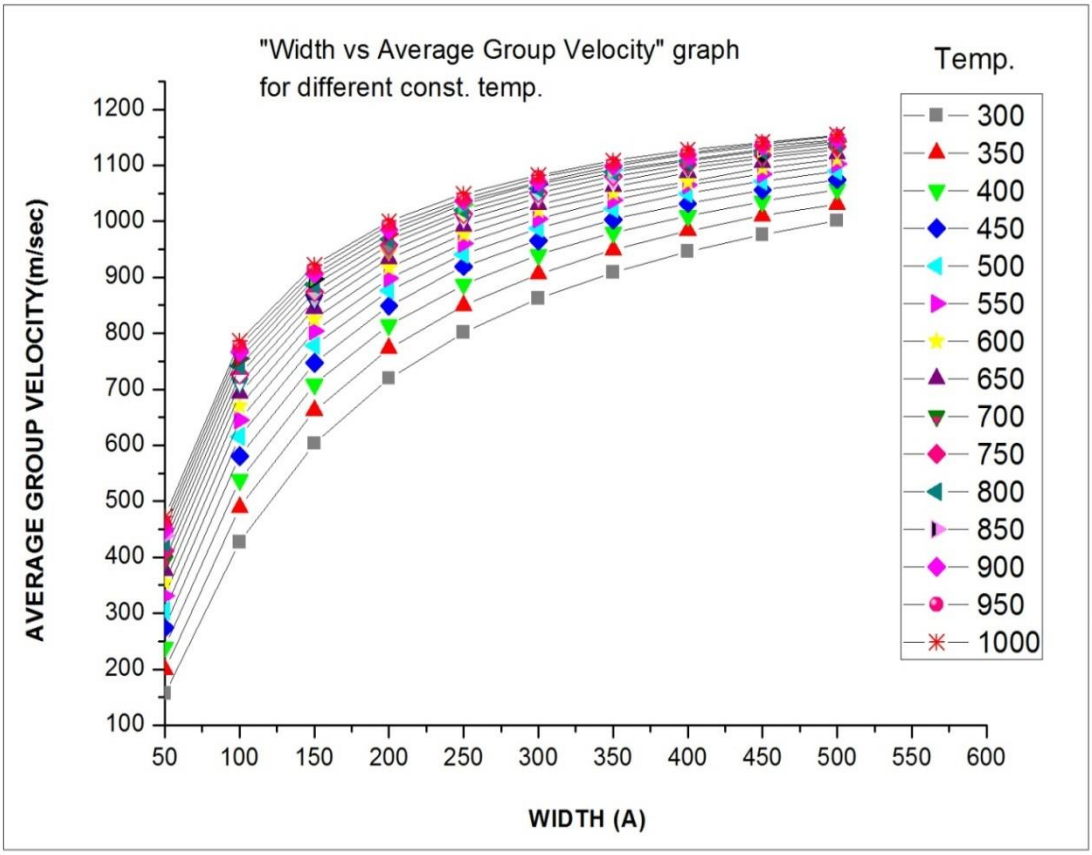


EXPLANATION:

The curves for different quantum well width show that on increasing the temperature the average group velocity increases sharply and then becomes almost flat. If we consider a particular quantum well width (say 100 Ang.) then the average group velocity will increase abruptly for low temperatures. Here in our calculation we have used the nine acoustic phonon modes to calculate the average group velocity. The average group velocity moves towards the bulk group velocity value if we go for the higher temperature region. Whereas, the average group

velocity becomes almost half the bulk value. The percentage change in average group velocity in lower width is more than the percentage change in the higher width values. It means that the lower width of the quantumwell structure has strong effect on the confinement of phonons and effectively decreases the group velocity. The quantum well with lower width values around 20 nm and smaller will be very effective for confinement of phonons. The transverse velocity for the bulk is 1266 ms-1 which reduces rapidly by decreasing the width of quantum well. For higher temperature and relatively thick quantum wells it approaches towards bulk value.

ii) **<u>Now the variation of average group velocity with width is shown in figure bellow:</u>**



<u>EXPLANATION:</u>

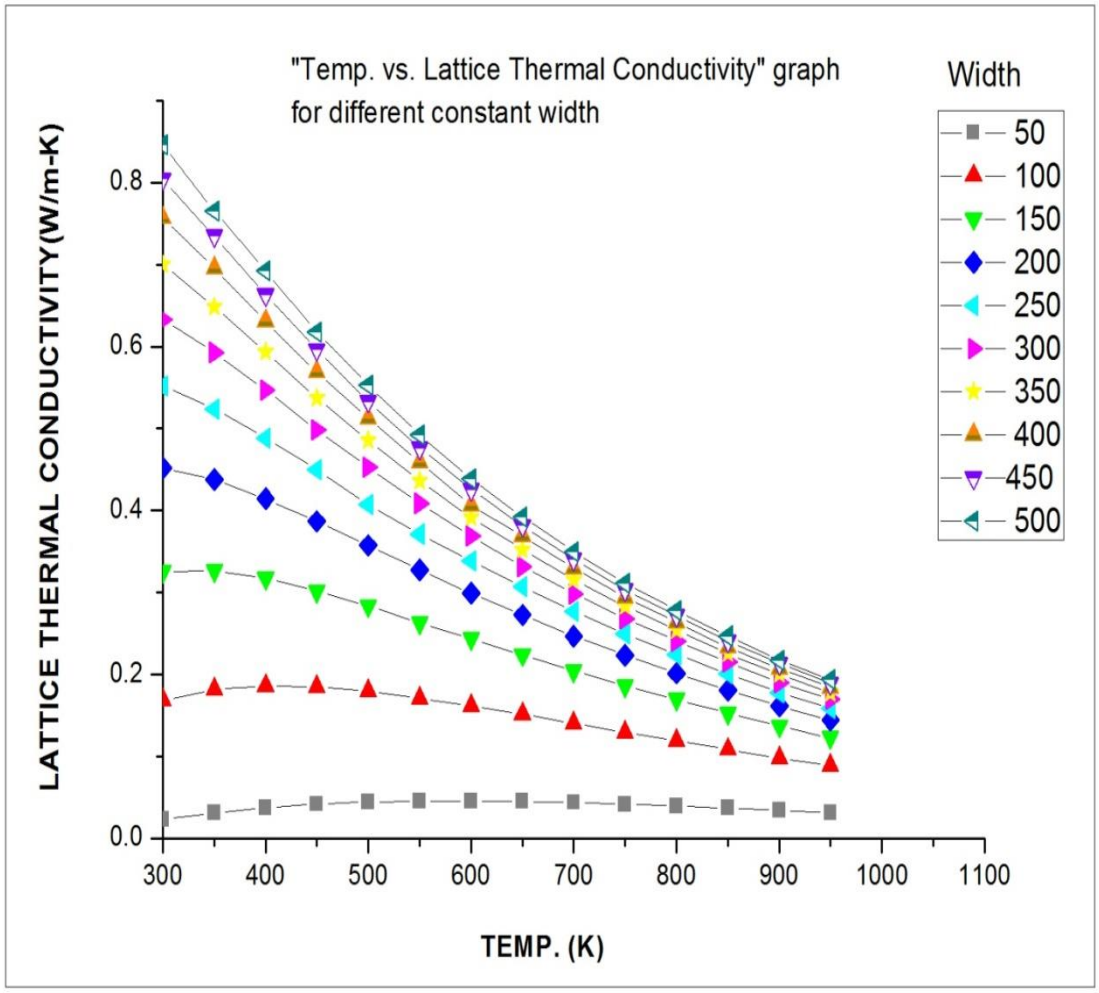
The value of average group velocity increases with increasing the value of width of the material and after certain value of width the value of average group velocity is almost constant. Also the value of average group velocity increases with increasing the value of temperature. Also we observe that the gap between two consecutive curves decreases with increasing the value of temperature. The slop of these curves decreases with increasing the value of width of the material for a constant value of temperature.

In this figure, it is clear that for a constant temperature, by increasing the width of quantum well the average group velocity increases. The increase in the average group velocity is comparatively very fast up to the value of width of quantum well 200 Angstrom and after that it becomes smaller. If we fix the
width of quantum well and for every increment of 100 K temperature, the change in group velocity is faster at lower temperatures as compared to the high temperatures and change is very small for the higher temperature range. It

means that in our bismuth telluride system the confinement effect will be dominant for the smaller quantum well width and for the small value of the temperature.

Lattice thermal conductivity (k_l):

i) The variation of lattice thermal conductivity with temperature



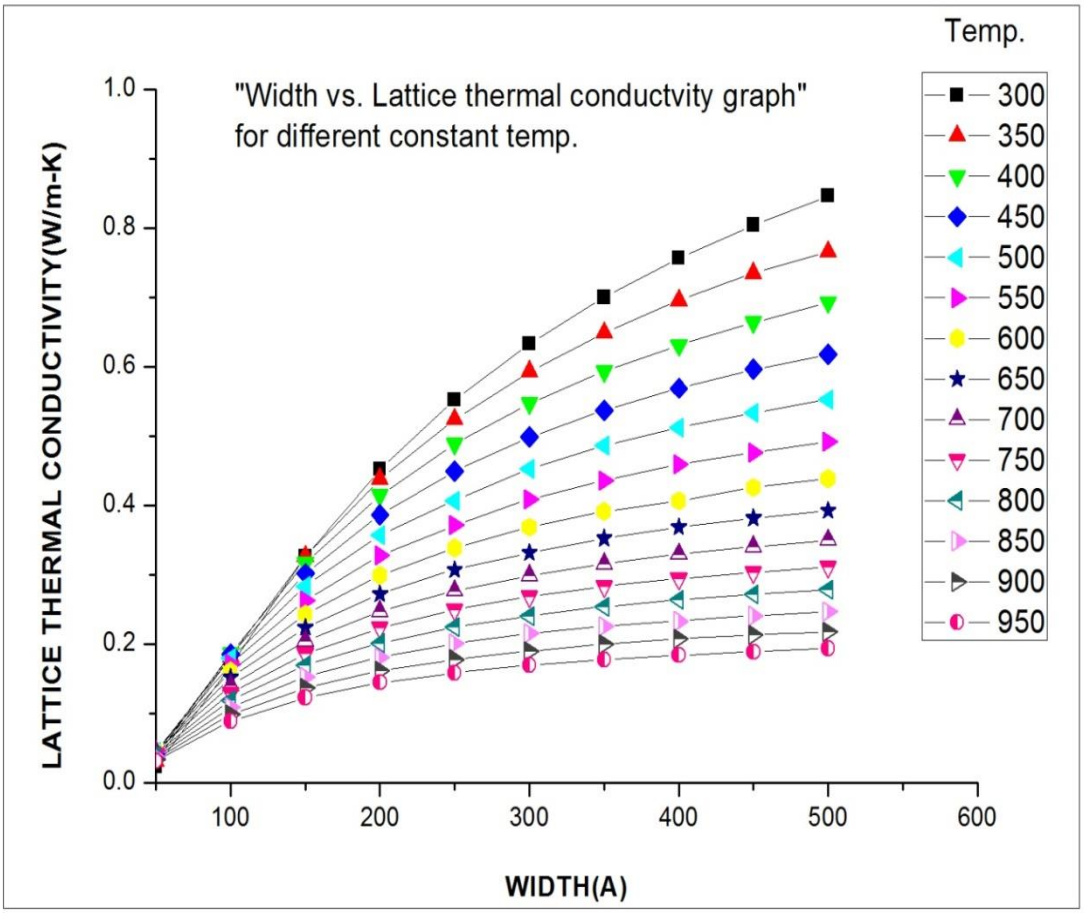
EXPLANATION:

The value of lattice thermal conductivity decreases with increasing the value of temperature for higher value of width of the material. We see that the width for 50Å, the value of lattice thermal conductivity is almost constant with increasing the value of temperature. It is obvious that the value of lattice thermal conductivity is very high for lower temperature for higher width. Also we observe that the gap between two consecutive curves decreases with increasing the value of width of the material.

There are two major scattering mechanisms, one is boundary scattering which is dominant for lower values of the width of quantum well whereas another one umklapp scattering is dominant for the higher temperature regions since it directly proportional to temperature. As we have discussed that the phonon confinement is effective at lower temperature and low value of width it means that boundary scattering should be large and umklapp will be small in this case. If we increase the value of temperature then there will be no effect on the boundary scattering but after a

certain temperature there will be dominance of umkalpp over the boundary scattering, and henceforth the relaxation rate will be very small and lattice thermal conductivity will decrease rapidly. Since lattice thermal conductivity is linearly proportional to temperature so in the figure it increases almost linearly and gets a maximum value. At this maximum point for the lower width quantum wells, we get the onset of umklapp scattering, which is very effective to decrease the relaxation time and hence forth due to combined effect of boundary scattering and the umklapp scattering, the lattice thermal conductivity decreases very fast for higher temperature regions. For the large width values, the boundary scattering is small and therefore the onset of umklapp scattering is at the lower temperature side so it is clear that we get a shift of peak on lower temperature region if we increase the width of quantum well. It is concluded that the peak in lattice thermal conductivity will occur at the lower temperature and when we take low dimensional material then the peak will shift towards higher temperature region.

ii) **Now the variation of lattice thermal conductivity with width is shown in figure bellow:**



EXPLANATION:

The value of lattice thermal conductivity increases with increasing the value of width of the material and after certain value of width of the material the value of lattice thermal conductivity is almost constant. We see that the value of lattice thermal conductivity is lower for lower value of temperature and width of the material. It is obvious that the value of lattice thermal conductivity is also increases with increasing the value of temperature. Also we observe that the gap between two consecutive curves increases.

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