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ВЕСТНИК

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A. Z. Issagulov[1], D. Belomestny[2], G. S. Shaiкhova[1],
V. V. Zhurov[1], L. Zh. Kasymova[1], G. Zh. Zhetimekova[3]

[1]Karaganda state technical university, Karaganda, Kazakhstan,
[2]University Duisburg-Essen, Duisburg and Essen, Germany,
[3]Karaganda state university, Karaganda, Kazakhstan.
E-mail: aristotel@kstu.kz, denis.belomestny@uni-due.de, shaikxova_2011@mail.ru,
zhurvitv@yandex.ru, l.kasymova_2017@mail.ru, jetimekova@mail.ru

FUNCTIONS OF ATOMS RADIAL DISTRIBUTION AND PAIR POTENTIAL OF SOME SEMICONDUCTORS MELTS

Abstract. The paper presents an estimate of the pair potential and the construction of the curves of the radial distribution of atoms in some melts of semiconductors such as germanium, silicon using the conducted studies in the framework of the density functional. The results of calculations of the potential for pair interaction in a germanium melt with the use of experimental data by V. M. Glazov and quantum potentials of pair interaction obtained by quantum chemical methods, respectively.

The temperature dependences of the radial distribution function of atoms in melts of selenium, tellurium, silicon, and germanium are studied theoretically. The results of the calculation of the radial distribution of atoms calculated by the molecular dynamics method are considered. If we assume that the position of the first maximum of the radial distribution curve of atoms in the melt corresponds to the shortest interatomic distance in atomic chains, then we must conclude that during the melting of a crystal this distance increases and a distorted crystal structure is obtained.

The potential of pair interplay in melts of germanium, silicon with usage of the conducted researches is estimated within the framework of a functional of density. The pair potentials are calculated under the electrostatic theorem of Gelman-Feynman, after finding of optimum electronic density conforming to equilibrium internuclear spacing interval.

Keyswords: pair potentials, radial distribution of atoms, semiconductor, structural factor atoms, molecular dynamics, density function, cluster structure.

Introduction. The structural difference of melts is conditioned by the difference of force fields, and consequently, by the difference of pair interaction potentials. It’s obvious that the difference in two structures semiconductors with different types of chemical bond is to effect the size and form of the pair potential, and decreasing the share of microzones indicated is to lead to changes reflecting structural transformations in the melt.

Methods. In this connection in the work, there has been evaluated the pair interaction in germanium, silicon melts using the studies carried out in the frames of density functional (pair potential are calculated by Gelman-Feynman electrostatic theorem after determining an optimal electronic density corresponding to the balanced internuclear distance). Usually, to calculate pair potential in liquids there are used three integral equations connecting with experimentally obtained structural factors, i.e. Bogolyubov-Born-Green equation, Percus-Yewik equation and hyperchain equation [1, 2].

From the analysis of these equations it follows that for calculation it's necessary to know the dependence of the structural factor $S(q)$ on the wave number. $S(q)$ is obtained from the experimental data on scattering electrons and neutrons X-rays, the upper limit being the wave number equal to 8-12Å. However, X-ray structural analysis data do not give a possibility to evaluate reliably the structural factor in the long-wave limit. At the same time the uncertainty in X-ray data evaluation by the way of extrapolation introduces a significant error in determining pair interaction potential.

In principle, the structural factor of these melts can be calculated using experimental data on the sound speed, density and heat capacity at constant pressure which was for the first time indicated by Landau and Lifshits [7], and to compare them with theoretical values $S(q)$. In figure 1, a and b, there are presented the results of pair interaction potential calculation in germanium melt using experimental data of V. M. Glazov and quantum potentials of pair interaction obtained by quantum-chemical methods, respectively. (Here, due to the fact that curves a and b are given in Angstroms, our results are also given in Angstroms for excluding additional errors, on one hand, and for the fact that the primary data were not tabulated, on the other hand.

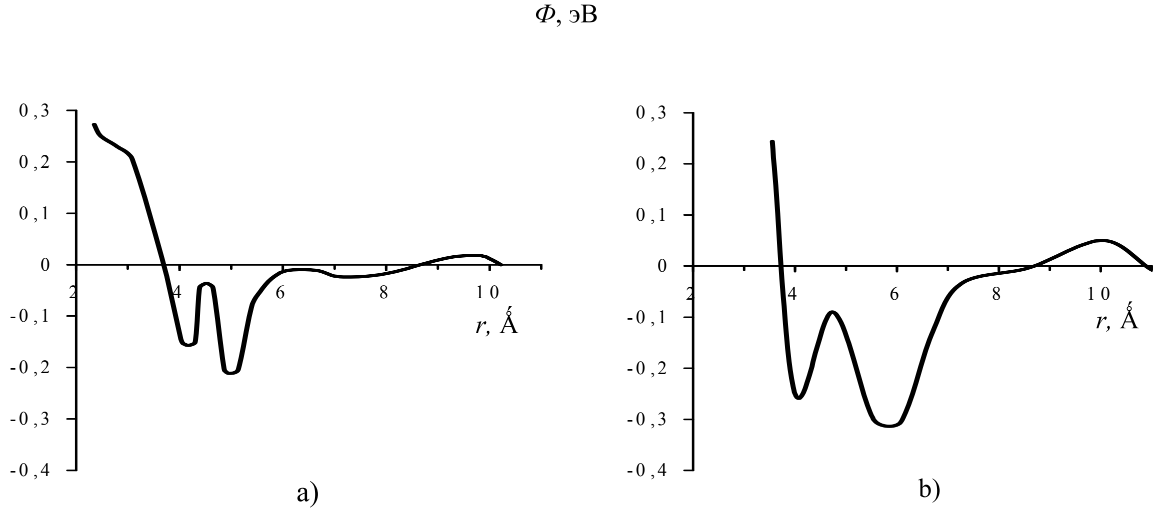

Figure 1 – Pair interaction potential in germanium melt:
a) – experiment; b) – calculation

As it is seen in the figure, at calculated values on $\Phi(r)$ dependence for germanium there is observed the potential minimum at r=3,7Å, which corresponds to the radius of the first coordination sphere. Besides, the potential abnormal behavior is observed at r=4,75Å, which corresponds to the radius of the second coordination sphere. It's worth noting that $\Phi(r)$ dependence in melted germanium is characterized by the presence of long-range oscillations.

Pair interaction potential calculation in melts using hyperchain equation lead to a similar result. It's worth noting that V. M. Glazov and his colleagues with the help of Percus-Yewik equations obtained $\Phi(r)$ dependences based on the data of the structural analysis. Based on the calculation results, the authors made a conclusion about a significant role of pair interaction potential dependence in liquid germanium on r. In figure 2 there is presented a pair interaction potential depending on inter-atom distance in silicon melt. It's obvious that this melt, as germanium, is characterized by pair interaction potential dependence near the point of melting and this dependence absence with large inter-atom distances [3, 5].

The results of the calculations carried out in germanium and silicon melts show that the structure reconstruction connected with breaking covalent bonds and their metallization don't' come to end completely at the melting temperature, but spreads to some temperature interval within the limits of which the processes comes to end. Structural differences observed in the process prove the process of post-melting.

Now let's consider the results of calculating the curves of atoms radial distribution computed by the method of molecular dynamics which algorithm is described in section 2.

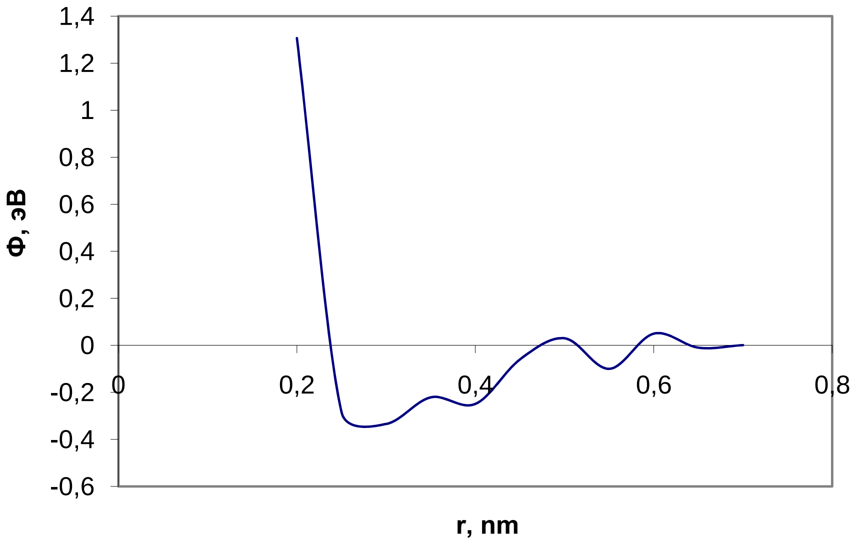

Figure 2 – Pair interaction potential in silicon melt at temperature 575 K

Near the melting temperature selenium is a viscous liquid, so in it there exist some structural elements of crystal modifications consisting of atomic chains or rings in a melt. This is proved by the position of the first two maxima of the atoms distribution curve in a melt shown in figure 3 at 500 K.

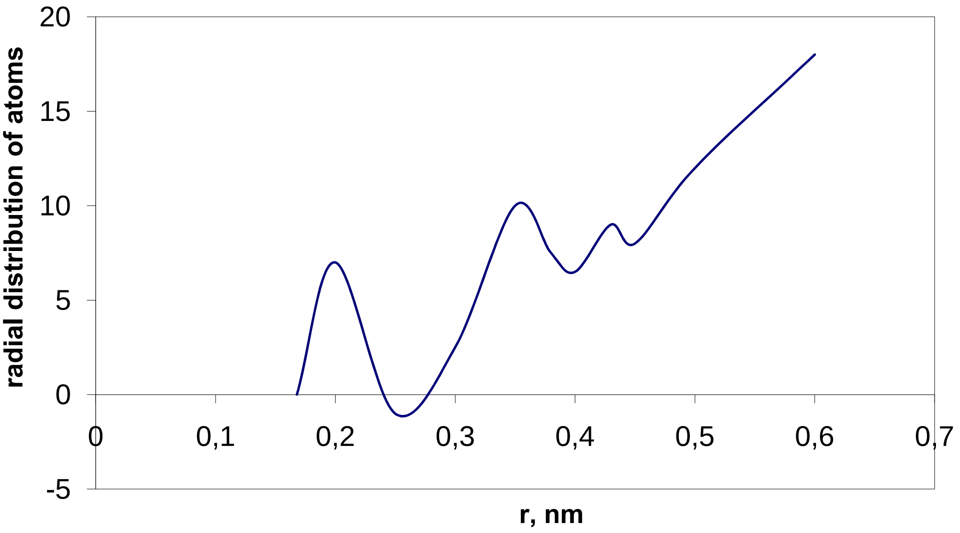

Figure 3 – Atoms radial distribution curve in selenium melt at temperature 500 K

This coincides with the value of inter-atom distances in screw chains typical for crystals. Molecular dynamics method using quantum potentials reproduces an experimental fact, and coordination numbers Z_1, Z_2 make 2,8 and 2,5, respectively. It's worth saying that the maximum at the distance 0,43 nm satisfies inter-atom distances in the screw chain, but, as shown in work [4], this can be referred to existing flat atomic chains. If in flat chains the shortest inter-atom distance is superseded about 0,2 nm and suppose their parallel location, then the following inter-atom distance is related to the zone of the second maximum of atoms radial distribution curve.

In figure 4 there is shown radial distribution curve at temperature 750 K, which has two clear maxima, and this may refer to Se_3 molecules that appear as a result of selenium chains atomic bonds breaking. The melt temperature increase to 740 K leads to increasing the shortest inter-atom distance, decreasing coordination number which in turn leads to disappearing an additional maximum at r_2=0,43 nm.

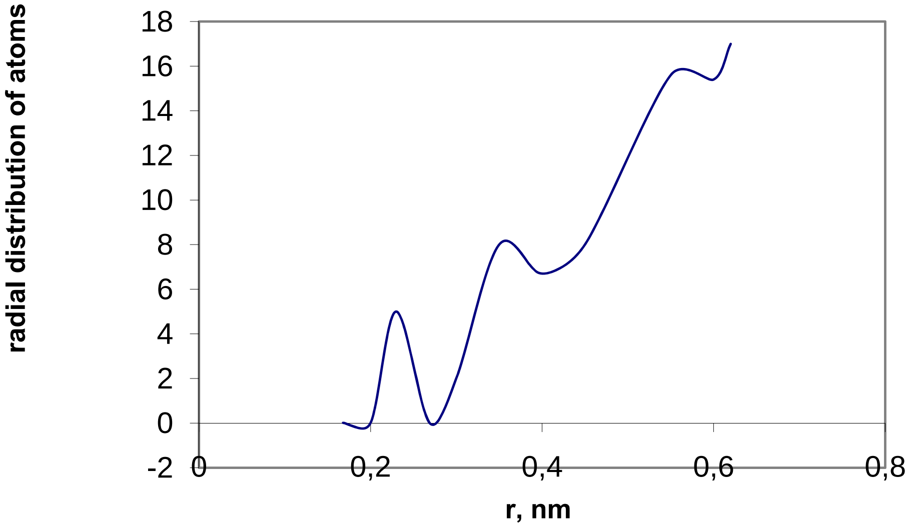

Figure 4 – Atoms radial distribution curve in selenium melt

A stable crystal modification of tellurium is a hexagonal modification which elementary cell is built of screw chains located along at the distances 0,2835; 0.4440 and 0,593 nm, where there are two atoms, and the shortest distance between four atoms of the neighboring chains is equal to 0.350 nm. Quantum calculations show that the bond between the atoms in the chain is covalent, conditioned by overlapping 5p-orbitals of impaired valent electrons, and between the chains there act Van der Walls forces, though in work [4, 6] there is expressed an opinion that the bond between atom chains is more complicated and to describe it we are to attract d-electrons.

In figure 5 there is presented atoms radial distribution curve calculated by molecular dynamics method at temperature 720 K.

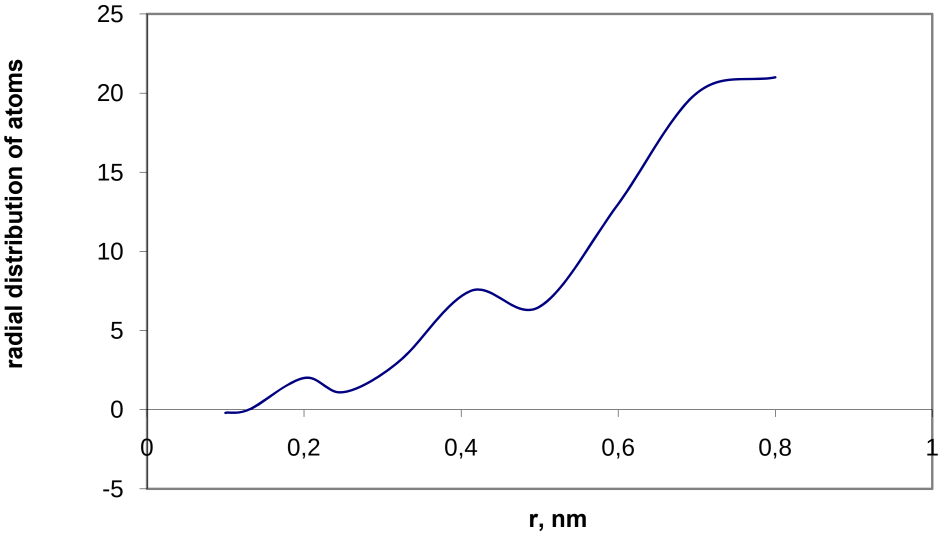

Figure 5 – Atoms radial distribution curve in tellurium meltat temperature 720 K

The calculations show that for this temperature the radial distribution curve has the following maxima: at 0,25; 0,413 and 0,78 nm, the coordination number being 2,3. This indicates that at melting tellurium there maintains its structure chain character.

The further heating of tellurium melt up to 880 K and higher seems not to lead to significant changes of its structure which is indicated by the flatness of atoms radial distribution curve.

Maxima positions of atoms radial distribution curve can be presented in such a way. Atoms distribution at temperatures 720 K and 780 K is close (figura 6). This can be explained by that in melt heating there take place rather minor changes of its short-order structure.

Maxima positions are close to the positions of the first and second maxima of atoms radial distribution curve at temperature 720ºC, however, the next maximum is very fuzzy.

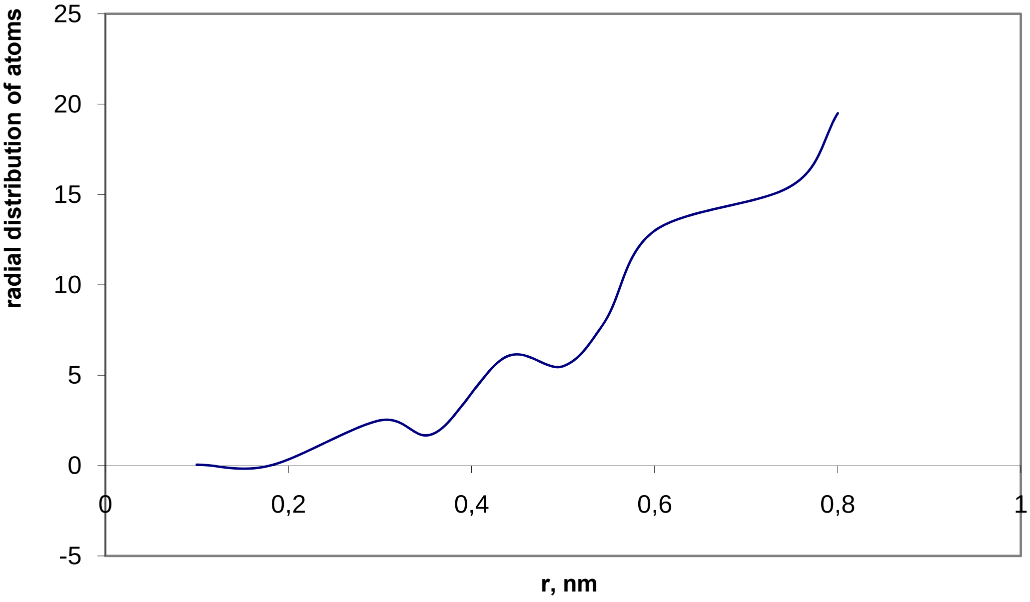

Figure 6 – Atoms radial distribution curve in tellurium melt at temperature 780 K

The value of the first coordination number of melted tellurium near the melting temperature permits to make a conclusion that its structural elements are rather atomic chains. if we suppose that the first maxima position of atoms radial distribution curve in the melt corresponds to the shortest inter-atom distance in atomic chains, then we can conclude that in crystal melting this distance increases and we obtain a distorted crystal structure.

If we suppose that in crystal melting inter-atom distances in atomic chains do not change, then atoms radial distribution in the melt can be presented as a sum of three Gauss curves which maxima are at 0,25; 0,413 and 0,78 nm, then the area under them will be equal to: Z_l = 1,9, Z_2 = 1,2, Z_3 = 7.2 at temperature 720 K, and at temperature 780 K Z_l = 1,8, Z_2 = 1,6 and Z_3 = 8,1.

This permits us to suggest a model of liquid tellurium structure presenting atomic chains differing in the value of the shortest distance. All the said permits to present the following picture of structural changes in tellurium. Tellurium melting leads to decaying bonds between atomic chains that build the crystal, but there maintains their existence in liquid state near the melting temperature. The melt heating to temperatures 780-850 K leads to partial decaying the chains and forming new structural elements.

Atoms radial distribution curve in liquid germanium is presented in figure 7, 8, there are also given the data of work [4, 10].

These data comparison with corresponding values for the distance r_l=0,294 nm, Z=4 shows that germanium melting is accompanied by significant changes in the short-order structure. Starting from the value of the first coordination number Z_1=8, V.K. Grigorovich suggested a model of liquid germanium based on the supposition that in melting there takes place its 4-valent electrons separation. Due to this, there uncover $3d^1$ –electron atom shells, chemically active $3d^6$ – orbitals of which are directed orthogonally. As a result of the directed interaction between the neighboring Ge^{4+} ions and collectivized valent electrons there forms a structure with the first coordination number $Z_1=8$. The first coordination sphere radius $r_1=0,28$ nm remains unchanged, and coordination number decreases from 7,62 to 7,25.

Atoms radial distribution curves behavior proves that in melts near $t_{пл}$ there exist statistically stable zones which atomic structure is close to that of the corresponding germanium crystals. The diffraction picture obtained experimentally proves the presence of such ordered zones which life duration ensures the possibility of coherent scattering of the incident X-ray radiation.

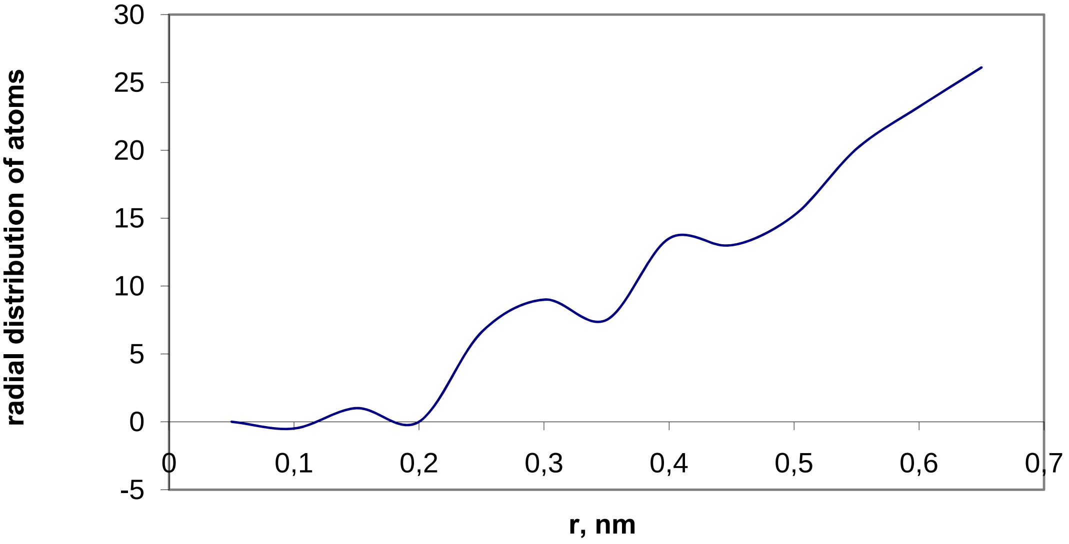

Figure 7 – Atoms radial distribution curve in germanium melt at temperature 1210 K

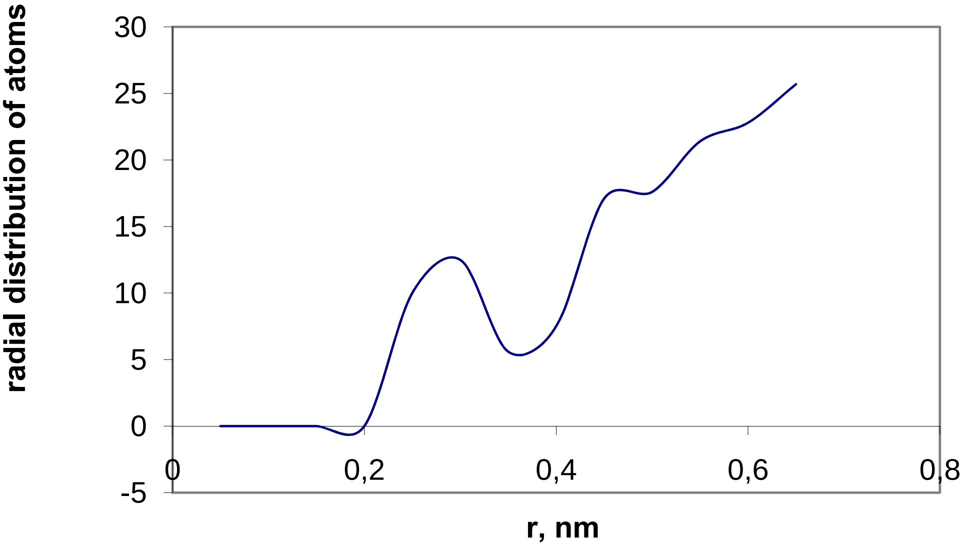

Figure 8 – Atoms radial distribution curve in germanium melt according to work [4] data

The first coordination sphere radius in the melt is 12.7 % more than in crystals, at the first maximum of atoms radial distribution curve in the melt with Z_1=5.7 there is the crystal first coordination sphere with Z_1=4,0. In the zone of the second coordination sphere in the melt with 10 atoms there are two crystal coordination spheres with 24 atoms. This proves changing the character of inter-atom bond in melting because it is the presence of mainly covalent bonds that defines low Z_1 value in crystals.

From comparison between r_i and Z_i for a melt and for a crystal presented in work [9] it follows that the latter is conditioned by prevailing structure consolidation due to Z_1 over its loosening due to increasing the shortest inter-atom distance. That's why we can make a conclusion about the similarity of the nearest neighbors in liquid germanium at 1210 K. It's worth noting that this conclusion is based on comparing four parameters of both structures, while supposition of neighbors' similarity in germanium melt follows only from that Z_1 in the melt determined by the method of asymmetric solving the first maximum of the radial distribution curve is equal to 8.

The short-order structure of the first type group corresponds well to the model of the fuzzy lattice, the second type group structure is somewhat more "loose" and seems to be conditioned by partial maintaining covalent bonds in a liquid melt. The melt heating leads to the gradual decaying the latter and consequently to the short-range order structure consolidation

The calculated curve of atoms radial distribution for silicon melt at the melting temperature is presented in figure 9, and the results of work [4, 8] in figure 10. Comparing the radial distribution curves in crystal and melted silicon are somewhat different.

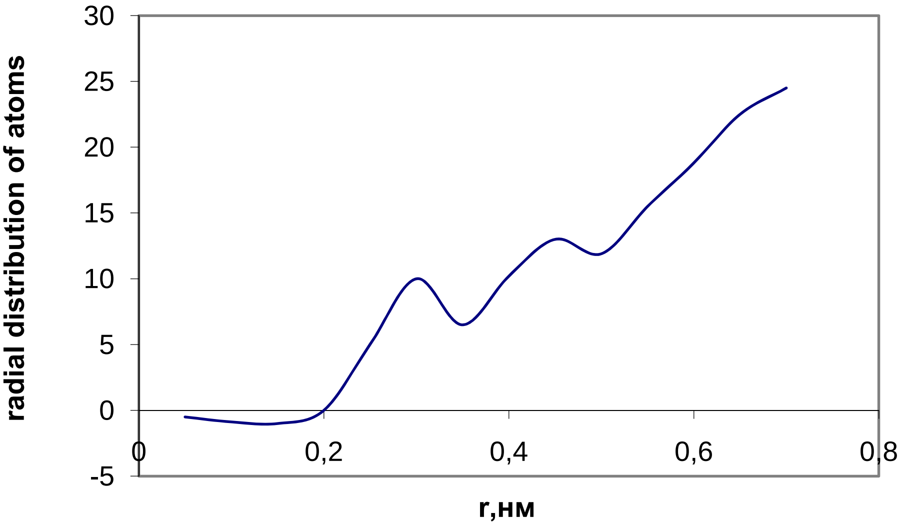

Figure 9 – Atoms radial distribution in silicon melt

In the distance range from 0,3 to 0,48 nm at the radial distribution in the crystal there are two maxima corresponding to the second and the third coordination spheres. In liquid silicon this range corresponds to the second fuzzy maximum, and these distances correspond to coordination numbers Z_1=6,8 and Z_2=12,8.

Results. The difference of radial distributions in crystal and melted silicon may prove that in crystal-melt transition there break covalent inter-atom bonds conditioning tetrahedral location of the nearest neighbors. "Loose" atom packing characterized on the atom radial distribution curve in the crystal by existing distances with a zero or close to zero radial density of atoms, gives place to their more dense packing in the melt.

Crystallographic and chemical similarity of germanium and silicon and the parameter value for the melt and the lattice r_l=0,52 make bases to try to describe liquid silicon structure, as well as germanium, by the model of the fuzzy s.c. lattice.

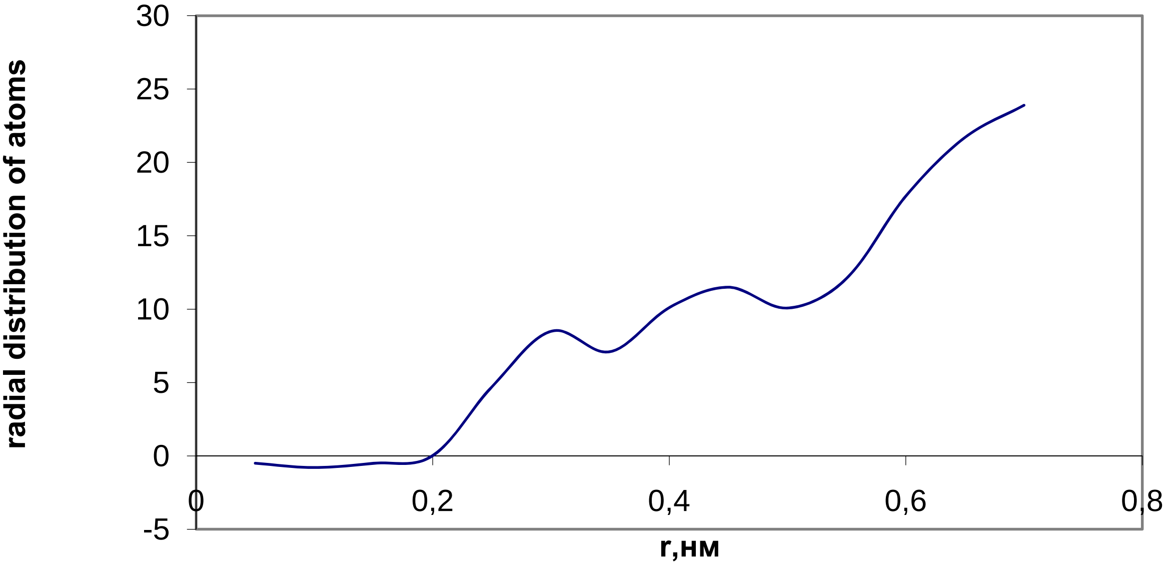

Figure 10 – Atoms radial distribution in silicon melt according to work [4] data

Discussion. The theoretical results obtained for the radial distribution of atoms in melts of selenium, tellurium, silicon, and germanium indicate that the semimetals and semiconductors are microheterogeneous. The results of calculations of the potential of pair interaction in germanium and silicon melts indicate that the structural rearrangement associated with the destruction of covalent bonds and their metallization does not end entirely at the melting temperature, but extends over a certain temperature interval within which the process ends.

А. З. Исағұлов[1], Д. Беломестный[2], Г. С. Шаихова[1], В. В. Журов[1], Л. Ж. Қасымова[1], Г. Ж. Жетімекова[3]

[1]Қарағанды мемлекеттік техникалық университеті, Қарағанды, Қазақстан,
[2]Дуйсбург-Эссен университеті, Дуйсбург және Эссен, Германия,
[3]Қарағанды мемлекеттік университеті, Қарағанды, Қазақстан

КЕЙБІР ЖАРТЫЛАЙ ӨТКІЗГІШ БАЛҚЫМАЛАРДЫҢ ЖҰПТЫҚ ПОТЕНЦИАЛЫ МЕН АТОМДАРДЫҢ РАДИАЛДЫ ҮЛЕСТІРІМ ФУНКЦИЯЛАРЫ

Анноатция. Жұмыста жұптық потенциал бағаланған және тығыздылық функционалы шеңберінде жүргізілген зерттеулердіпайдаланып, германий, кремний сияқты жартылай өткізгіштердің кейбір балқымаларында атомдардың радиал үлестірімінің қисықтарысалынған. В. М. Глазовтың эксперименттік деректерін қатыстыру арқылы германий балқымасындағы жұптық өзара әрекеттесу потенциалын есептеудің нәтижелері және сәйкесінше кванттық-химиялық әдістермен алынған, жұптық өзара әрекеттесудің кванттық потенциалдары келтірілген.

Теориялық түрде селен, теллури, кремний және герман балқымаларындағы атомдардың радиалды үлестіру функциясының температуралық тәуелділігі зерттеледі.Молекулярлық динамика әдісімен есептелген атомдардың радиалды қисықтарын есептеу нәтижелері қарастырылған. Егер балқымадағы атомдардың радиал үлестірімі қисығының бірінші максимумының орны атомдық тізбектердегі атом аралық ең қысқа қашықтыққа сәйкес келетінін болжасақ, онда кристалл балқыған кезде бұл ара қашықтық ұлғаяды және бұрмаланған кристалдық құрылымы алынады деген қорытынды жасау керек..

Тығыздық функционалының шеңберінде германий және кремний балқымаларының атомдардың жұптық әсерлесу потенциалдары есептелген. Жұптық потенциалдар тепе-теңдік аралықтарды тапқан соң Гельман–Фейманның электростатистикалық теоремасы арқылы табылады.

Түйін сөздер: жұптық потенциалдар, атомдардың үлестірім функциясы, жартылай өткізгіштік, функционал тығыздығы, атомдар, молекулалық динамика, кластерлік құрылым.

А. З. Исагулов[1], Д. Беломестный[2], Г. С. Шаихова[1], В. В. Журов[1], Л. Ж. Касымова[1], Г. Ж. Жетимекова[3]

[1]Карагандинский государственный технический университет, Караганда, Казахстан,
[2]Университет Дуйсбург-Эссена, Дуйсбург и Эссен, Германия,
[3]Карагандинский государственный университет, Караганда, Казахстан

ФУНКЦИИ РАДИАЛЬНОГО РАСПРЕДЕЛЕНИЯ АТОМОВ И ПАРНОГО ПОТЕНЦИАЛА НЕКОТОРЫХ РАСПЛАВОВ ПОЛУПРОВОДНИКОВ

Аннотация. В работе приведена оценка парного потенциала и построение кривых радиального распределения атомов в некоторых расплавах полупроводников, таких как германий, кремний с использованием проведенных исследований в рамках функционала плотности. Приведены результаты расчетов потенциала парного взаимодействия в расплаве германия с привлечением экспериментальных данных В. М. Глазова и квантовые потенциалы парного взаимодействия, полученные квантовохимическими методами, соответственно.

Теоретически исследованы температурные зависимости радиальной функции распределения атомов в расплавах селена, теллура, кремния и германия. Рассмотрены результаты расчета кривых радиального распределения атомов, рассчитанные методом молекулярной динамики. Если предположить, что положение первого максимума кривой радиального распределения атомов в расплаве соответствует кратчайшему межатомному расстоянию в атомных цепях, то следует сделать заключение, что при плавлении кристалла это расстояние увеличивается и получается искаженная кристаллическая структура.

Потенциал парного взаимодействия в расплавах германия, кремния с использованием проведенных исследований оценивается в рамках функционала плотности. Парные потенциалы вычисляются по электростатической теореме Гельмана–Фейнмана, после нахождения оптимальной электронной плотности, соответствующей равновесный межъядерный интервал.

Ключевые слова: парные потенциалы, радиальные распределения атомов, полупроводник, функционал плотности,структурный фактор, атомы, молекулярная динамика, кластерная структура.

Information about authors:

Issagulov A. Z., Karaganda state technical university, Karaganda, Kazakhstan; aristotel@kstu.kz; https://orcid.org/0000-0003-2174-9072

Belomestny D., University Duisburg-Essen, Duisburg and Essen, Germany; denis.belomestny@uni-due.de; http://orcid.org/0000-0002-9482-6430

Shaikhova G. S., Karaganda state technical university, Karaganda, Kazakhstan; shaikxova_2011@mail.ru; https://orcid.org/0000-0002-2036-3023

Zhurov V. V., Karaganda state technical university, Karaganda, Kazakhstan; zhurvitv@yandex.ru; https://orcid.org/0000-0002-4413-8584

Kasymova L. Zh., Karaganda state technical university, Karaganda, Kazakhstan; l.kasymova_2017@mail.ru; https://orcid.org/0000-0002-4696-867X

Zhetimekova G. Zh., Karaganda state university, Karaganda, Kazakhstan; jetimekova@mail.ru; https://orcid.org/0000-0001-8101-4065

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