Available online at www.sciencedirect.com

ScienceDirect

Physics Procedia 72 (2015) 338 – 341

Physics Procedia

Conference of Physics of Nonequilibrium Atomic Systems and Composites, PNASC 2015, 18-20 February 2015 and the Conference of Heterostructures for microwave, power and optoelectronics: physics, technology and devices (Heterostructures), 19 February 2015

# Molecular-Dynamics Study Melting Aluminum at High Pressures

S.A. Gubin[a]*, I.V. Maklashova[a], A.A. Selezenev[a,b], S.A. Kozlova[a]

[a]*National Research Nuclear University MEPhI, Kashirskoye shosse 31, Moscow 115409, Russia*
[b]*Russian Federal Nuclear Center All-Russian Research Institute of Experimental Physics, Sarov, Russia*

**Abstract**

The dependence of the melting temperature versus the pressure under static conditions and under shock-wave compression of aluminum was calculated by molecular-dynamic modeling technique. The Morse potential and EAM potential (embedded atom method) was used for the interatomic interaction for the solid and liquid phases of aluminum. The calculations show a change of crystal structure of aluminum close to the melting range static compression and compression in the shock wave. Melting point was determined by analysis of the radial distribution function and the standard deviation of the atoms with the visualization of crystal structure. The results of molecular dynamics calculations are consistent with experimental data on the compressibility of the shock wave up to 200 GPa. Static melting results are consistent across the field of experimental data up to 30 GPa. A short-term compression in the shock wave, accompanied by the increase of entropy can be leads to overheating nonequilibrium substances. Under these conditions, the melting temperature under static and shock compression may be different from each other. However, the calculations showed on pressure in the shock wave 122 GPa aluminum melting occurs at temperatures close to the melting temperature in static conditions.


Peer-review under responsibility of the National Research Nuclear University MEPhI (Moscow Engineering Physics Institute)

*Keywords:* molecular-dynamic simulation, shock wave, the intermolecular interaction potential, melting line

* Corresponding author. Tel.: +8-495-788-56-99(9035).
*E-mail address:* sagubin@mephi.ru


Peer-review under responsibility of the National Research Nuclear University MEPhI (Moscow Engineering Physics Institute)
doi:10.1016/j.phpro.2015.09.106

**Nomenclature**

| | |
|---|---|
| $P$ | pressure |
| $T$ | temperature |
| $V$ | specific volume |
| $E$ | internal energy |
| $U$ | mass velocity |

## 1. Introduction

Aluminum is the effective component of structural and energetic materials exposed to high loads, including high pressures and temperatures. The prediction of thermophysical properties of Al in a wide range of pressure and temperature is extremely important to prevent of accidents and efficiency of devices. It is therefore important to know thermal properties of solid and liquid aluminum at high pressures and temperatures and the area of melting aluminum in Shock wave.

Molecular dynamic method was used in [1–7] for studying the melting of aluminum. Calculations just of the shock wave was carried out in [2-4] without determining the melting line of Al in static conditionals for comparison of melting parameters. The melting point in shock wave [1,4] was determined by the intersection the melting line and the numerical shock adiabat without analyzing the structure and phase state of aluminum. However, the approach [1] does not take into account such features of shock wave as a short-term compression accompanied by the increase of entropy, nonequilibrium overheating of substances. Only modeling of static melting is made in [5-7]. In details the crystal structure at melting area in a shock wave wasn't investigated. Therefore, only direct molecular dynamics simulations of compression in shock waves together with the analysis of the structure of aluminum can provide close to the experimental value of the melting point.

## 2. Procedure of molecular dynamics simulation

The computer code SageMD [8] used to molecular dynamics (MD) simulation of the melting of aluminum under shock compression and static conditions. The computational MD cell of aluminum presented in the form of a cube. In the initial state of the lattice structure of aluminum - face-centered cubic, lattice period 4.050 Å. The unit cell of the crystal contains 4 aluminum atom. The computational MD supercell is constructed from 10 unit cells in each direction and consisted of 4000 atoms of aluminum. In carrying out MD simulations in all three spatial directions used periodic boundary conditions. MD simulation allows to visualize the structure of aluminum on the atomistic level and to calculate the properties of the material by the shock wave heated. The visualization tools allow fixing the atomic structure, the distribution of atoms in a microvolume and to determine the phase state of matter. The change of the atoms location in the computational cell during melting clearly indicates the loss of near and long-range order. The use of the radial distribution function and mean square deviation in the MD modeling allows to analyze the destruction of condensed matter behind the shock wave front or in static conditionals.

The Morse potential and EAM potential (embedded atom method) was used for the interatomic interaction for the solid and liquid phases of aluminum.

To describe the adiabat of shock compression of a solid by one-dimensional flat wave was used Rankine - Hugoniot relationship for change in the internal energy $E$ as a function of the pressure $P$ and the specific volume $V$ (physical values with the subscript "0" correspond to the parameters of the medium in front of the shock wave)

$$E - E_0 = \frac{1}{2}(P + P_0)(V - V_0).$$

It enable to calculate all thermodynamic properties of matter along the shock adiabat. Implemented in the SageMD code [8] the Hugoniotstat method [9] was used for MD simulation of shock compression of aluminum crystal. The

calculated shock adiabat (the dependence of the shock wave velocity on the mass velocity behind the wave front, the dependence of the pressure of aluminum shock compression on compression ratio of the material) of aluminum was compared with the experimental data [10]. It can be seen from Fig. 1 that the calculated data (lines) are in excellent agreement with experimental data (markers) [10] as thermophysical and so wave characteristics of shock wave compression of aluminum over the entire range of pressure, as with a small compression ratio, and so at extremely high.

For comparison of values of pressure and temperature on shock adiabat with areas of phase stability of aluminum melting parameters at static compression are shown [5-7, 12-14] in fig. 2. Line in fig. 2 is calculated values of pressure and temperature shock compression in this study, markers as red rhombus are state melting obtained in this work, markers [11] are measured values of pressure aluminum melting in the shock wave. It can be seen from Fig. 2 that the calculated data (red rhombus markers) are in good agreement with experimental data [11-13].

## 3. Discussion

Fig. 2 shows that the shock wave parameters at pressures up to 100 GPa lie in the region of existence of solid aluminum. The experimental data [11], corresponding to the melting of aluminum in the shock wave, are in good agreement with a bend at the calculated dependence of pressure behind the shock wave front. This indicates that the melting region of shock-compressed Al predicted correctly. Shock adiabat parameters at high pressures above 120 GPa, most likely lie in the existence of liquid aluminum. The MD simulation results indicate the melting of aluminum in shock wave at a pressure of about 122 GPa and a temperature of 4200 K. Calculations have shown that static aluminum melting occurs at a temperature T = 4100 K at a pressure P = 120 Gpa. Accordingly aluminum melting in shock wave occurs at temperatures close to the melting temperature in static conditions.

Under loading substance to a pressure near the intersection of the melting curve and the shock adiabat experimentaly observed interesting mode [15]. The metal is melted in the shock wave or wave unloading. Then there is a smooth pressure drop in substance (unloading) and it goes to under the melting curve, i.e. to the solid phase. In our calculations, this region corresponds to a pressure of 120-140 Gpa. Theoretically should occur rapid solidification of the melt, but to realize the solid phase must be amorphous. To investigate this region need detailed visualization of the crystal structure on the shock wave.

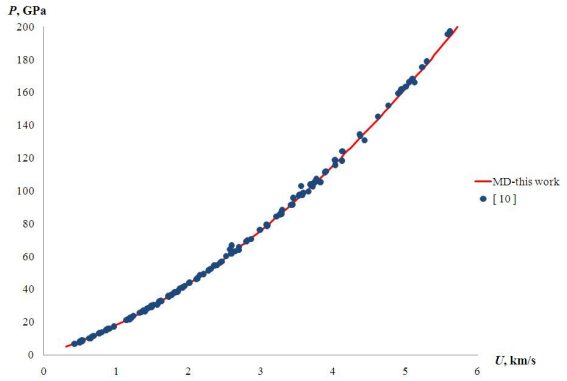


Fig. 1. The pressure of the shock wave velocity on the mass velocity behind the wave front. Line is this work, markers is experimental data [10].

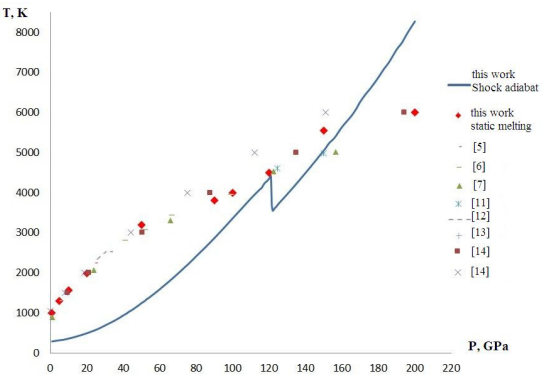


Fig. 2. The Hugoniot adiabat on the phase diagram Al. Line – calculated pressure vs temperature shock compression, markers as red rhombus – state melting in this work. Markers [11] – measured melting pressure in the shock wave, markers [5-7, 11-14] – the melting point of aluminum with static compression.

## 4. Conclusion

By the MD simulation using Hugoniotstat techniques properties of aluminum in the solid and liquid phases and the temperature dependence of pressure in the shock wave were calculated.

The characteristic bend on the obtained crystal temperature dependence on the pressure of the shock wave is observed at pressure of 115-122 GPa. The nature of the bend on the curve may indicate the presence of a phase transition in the crystal structure of aluminum (melting) in this range of temperatures and pressures. Visualization of the crystal structure and the atomic radial distribution function indicate that the arrangement of atoms has not got order at these temperatures and pressures. This configuration can be interpreted as the aluminum melting.

The MD outcomes were compared to other experimental and theoretical data. Comparison of the results obtained in this work with published results of simulation of temperature static melting point of aluminum, as well as experimental data of static melting and experimental melting parameters in shock wave on the pressure shows their mutual consistency. The calculations showed on pressure in the shock wave 122 GPa aluminum melting occurs at temperatures close to the melting temperature in static conditions. In the region of 120-140 GPa aluminum may be amorphous.

## References

[1] Jeong JW, Lee IH, Chang KJ. Molecular-dynamics study of melting on the shock Hugoniot of Al. *Phys Rev B.* 1999; 59: 329-333.

[2] Selezenev AA, Golubev VK, Aleinikov AY, Butnev OI, Barabanov RA, Voronin BL. Molecular Dynamics Simulation of Shock Wave Compression of Metals. *Proc. of Int. Conf.* «Shock Compression of Condensed Matter» (SCCM) 2001; USA, Atlanta: 374-377.

[3] Ju Y, Zhang Q, Gong Z, Ji G, Zhou L. Molecular dynamics simulation of shock melting of aluminum single crystal. *Journal of Applied Physics* 2013; 114 (9): 093507 .

[4] Gubin SA , Maklashova IV , Selezenev AA , Kozlova SA , Demidenko TS. Molecular dynamics simulation and visualization of melting aluminum crystal in shock wave. *Scientific Visualization* 2014. 6 (5): 14-23.

[5] Botyachkova AI, Gubin SA, Sokolova IL, Karpinskiy GG. Molecular dynamics simulation of melting aluminum in macrostate at high pressure. *Nuclear physics and engineering* 2013; 4 (5): 423-424. (*in Russian)*

[6] Starikov SV, Stegailov VV. Atomistic simulation of the premelting of iron and aluminum: Implications for high-pressure melting-curve measurements*. Phys Rev B* 2009; 80: 220104.1-220104.4.

[7] Bouchet J, Bottin F, Jomard G, Zérah G. Melting curve of aluminum up to 300 GPa obtained through ab initio molecular dynamics simulations*. Phys Rev B* 2009; 80: 094102.1- 094102.5.

[8] Selezenev AA, Aleynikov AYu, Gantchuk NS, Yermakov PV, Labanovski JK, Korkin AA. SageMD: molecular-dynamic software package to study properties of materials with different models for interatomic interactions. *Computational Material Science* 2003; 28:107-124.

[9] Selezenev AA, Aleynikov AYu, Ganchuk NS, Ermakov PV, Ganchuk SN, Aidun JB, Thompson AP. Shock Compression Calculation of RDX and PETN Molecular Crystals using Hugoniostat Method. *Shocked Compression of Condensed Matter, AIP Conf. Proc* 2009; 821: 1195.

[10] Shock Wave DataBase. Available at: http://www.ihed.ras.ru/rusbank/ (accessed: Juny 7, 2014).

[11] Shaner JW, Brown JM, McQueen RG. Melting of metals above 100 GPa. *Materials Research Society Symposia Proceedings* 1984; 22: 137–141.

[12] Baker EL,Capellos Ch. *Jaguar procedures for detonation properties of aluminized explosives*. U.S. ARMY TACOM-ARDEC Picatinny Arsenal, New Jersey 07806.

[13] Boehler R, Ross M. Melting curve of aluminum in a diamond cell to 0.8 Mbar: implications for iron. *Earth Planet Sci Lett* 1997; 153: 223.

[14] Moriarty JA, Young DA, Ross M. Theoretical study of the aluminum melting curve to very high pressure. *Phys Rev B* 1984; 30: 578-588.

[15] Drennov OB. Dynamic loading of solids with a negative slope of the melting curve. *Technical Physics* 2013; 58 (9): 1284-1287.