MOLECULAR DYNAMICS SIMULATION OF CRYSTAL MELTING ALUMINUM AT HIGH PRESSURES

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Abstract: The dependence of melting temperature vs. pressure under static conditions and under shock-wave compression of aluminum was calculated by molecular-dynamic modeling technique. The Morse potential was used for the interatomic interaction for the solid and liquid phases of aluminum. The Hugoniot adiabats, changes of the crystal structure, and the temperature of shock heating were determinated. The results of molecular-dynamic calculations with high accuracy are consistent with the experimental data on shock wave compressibility. The range of aluminum melting under shock-wave compression was selected. The obtained results were compared to the experimental and theoretical data for determining reliable parameters of melting. It is calculated that at pressure of 122 GPa, the melting of aluminum in shock wave occurs at a higher temperature than the melting under static conditions.

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

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Received November 1, 2014

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