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Stastistical-thermodynamic study of nonequilibrium phenomena in three-dimensional anharmonic crystal lattices. I: Microscopic basic equations. (English) Zbl 1122.82316

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Summary: Microscopic basic equations for analyzing nonequilibrium phenomena in three-dimensional anharmonic crystal lattices at finite temperatures are self-consistently derived from the Liouville equation by adopting both independent particle approximation and Gaussian approximation. The model prescribed by the basic equations can be regarded as the dynamical version of the self-consistent Einstein model, and is valid in a wide temperature range including the melting point. Thermal equilibrium states of several fcc and bcc crystals are also analyzed by using the basic equations. Singularities in the temperature dependences of the nearest-neighbor distance and the amplitude of thermal vibration at the melting point are found, and Lindemann's law is examined. The results obtained here will be utilized in the analyses in the following papers of the present series.

MSC:

82C99 Time-dependent statistical mechanics (dynamic and nonequilibrium)
80A20 Heat and mass transfer, heat flow (MSC2010)
82D25 Statistical mechanics of crystals

Keywords:

nonequilibrium phenomena; three-dimensional anharmonic crystal lattice; Liouville equation; melting

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