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Exact thermodynamic calculation of a monatomic system and its ideal glass transition on a new recursive lattice formed by cubic units
RAN HUANG, PURU GUJRATI, The Univeristy of Akron — A many-body Ising lattice model is used to represent monatomic systems and is solved exactly on a new recursive lattice with the aim to study the metastability in supercooled liquids and the ideal glass transition. Interactions between particles farther away than the nearest neighbor distance are taken into consideration. The Ising model is antiferromagnetic in nature so that its ordered phase represents an alloy-type crystal of alternating species (A-B or particle-void). The new recursive lattice appears quite reliable to represent a cubic lattice. Thermal properties including free energy, energy and entropy of the ideal crystal and supercooled liquid state of the model are calculated. The computation results show a first order melting and second order ideal glass transition (entropy crisis) in the supercooled liquid phase. The effects of different energy terms on the two transitions are studied. We also study the defects in the ideal glass, supercooled liquid and the crystal to support the theory that a glass can be treated as a highly defective crystal.

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