Supplementary Material

Freezing and melting of water and ice: Theoretical modeling in nanoscale

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Part 1: Force-Heat equivalence energy density principle

The core idea of the Force-Heat equivalence energy density principle[1, 2] is that both strain energy and heat energy can make the failure of materials. From the perspective of material failure, there is a certain equivalent relationship between them, because they have different contributions to material failure. A great many experiments and simulations indicate that the obvious softening effect on material with the temperature increases, and the mechanical properties show a decreasing trend[3, 4]. In addition, with the increasing temperature, the resistance of the lattice to dislocation slip will decrease.[5] According to Gao's work[6], the pre-melting temperature of the grain boundary would decrease under the action of external stress. And the dislocation system would jump over the barrier due to the thermal fluctuations, which precipitates the failure of the material[7]. Thus, both external stress and heat energy can contribute to the failure of materials[8]. As known, it required sufficient energy to overcome the bonding forces between the atomic lattices, which is due to the collective

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action of atoms accompanying the external stress and heat energy.[9] Their contributions to the failure of materials are different, which means there is a certain equivalence between them. From the perspective of microscopic, the atomic or chemical bond will break under the action of the temperature or external force. Whereas the external force (strain energy) would make partial chemical bonds break, the temperature (heat energy) would result in all the chemical bonds breaking[10]. Therefore, their effect on material failure is not exactly the same and these energies are not numerically equal, but rather the equivalent effect on material failure. It can be concluded that there is an equivalent coefficient between strain energy and heat energy.

Different materials have different capacities to store energy, and the energy of any material is limited. There are many scholars who studied material behavior under the action of force-heat because it is so complex[11]. Combining the above analysis and considering the influences of temperature, Li[1] put forward the Force-Heat equivalence energy density principle that the maximum energy storage density consists of strain and heat energy. In order to predict the material behavior on this condition and can easily and conveniently use the established model, we started the research that assumes a linear relationship which the simplest way. Based on this hypothesis, Li has developed a series of temperature-dependent theoretical models without fitted parameters for advanced ceramics and their composites[12, 13], polymers and their composites[14, 15], metals[10, 16]. Furthermore, this principle has been successfully extended to characterize the size effect of nanometals and carbon nanotubes.[17-19] Furthermore, this principle has been successfully applied to temperature, and pressure-dependent mechanical properties of various material systems.

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