Homogenous Melting Mechanism in Superheated Crystals

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Homogeneous melting, i.e., without nucleation at surfaces, is a long-standing topic which has received much attention in recent years. It can be studied by molecular dynamics modeling where the position of every atom is traced at each instant, as a crystal transforms from solid to liquid. Relying on such simulations, relevant for aluminum, it is shown that the thermal fluctuation initiating homogeneous melting in a superheated state is an aggregate typically with 6-7 interstitials and 3-4 vacancies. This mechanism differs from those that have traditionally been proposed, e.g. instability under shear or formation of dislocations. The detailed study of the creation, motion, and annihilation of individual lattice defects in a large number of simulations gives the following picture. Vacancy-interstitial pairs are created through thermal fluctuations. Normally such pairs rapidly annihilate, but sometimes a pair separates instead. Interstitials, being more mobile than vacancies, migrate through the lattice. When two interstitials come close, they usually form a bound system, which may then bind one or two additional migrating interstitials. In the next step, interstitial-vacancy pairs are created close to the interstitial aggregate. In most cases, such vacancies rapidly annihilate with interstitials in the aggregate, but occasionally a local defect structure is formed that contains several interstitial-vacancy pairs, in addition to the original interstitials. Also, this configuration may return towards a more ordered lattice, but when it has more than about ten point defects, we find that it usually continues to grow. Thus, complicated statistical fluctuations are essential in the several steps of the melting mechanism. Through explicit calculations of elastic moduli, it is confirmed that the lattice has not yet become unstable under shear when homogeneous melting takes place. This contribution elaborates on recent results by M. Forsblom and G. Grimvall: *Nature Materials* **4**, 388 (2005); *Phys. Rev. B* **72**, 054107 (2005).