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Homogeneous melting of superheated crystals MATTIAS FORSBLOM, Royal Institute of Technology, AlbaNova University Center, Department of Physics, Theory of materials, Stockholm, Sweden, GÖRAN GRIMVALL, Royal Institute of Technology, AlbaNova University Center, Department of Physics, Theory of materials, Stockholm, Sweden — Homogeneous melting of crystals (i.e. not initiated at a surface) has been studied in many works but the detailed mechanism is still not well understood. We have carried out molecular-dynamics simulations for a realistic case (fcc Al) with the interaction of Ercolessi and Adams to thoroughly track the microscopic path of the solid-to-liquid transition. Due to periodic boundary conditions the surface-melting mechanism is suppressed and melting occurs in a superheated state at a temperature about 30 % above the equilibrium melting point. We find that the thermal fluctuation initiating the melting process is an aggregate of point defects, with typically 6-7 interstitials and 3-4 vacancies, which acts as a nucleation site for the growth of the liquid phase. This picture differs from those previously proposed in that the configuration initiating melting involves much fewer particles. Other mechanisms are not necessarily false but we have identified the smallest defect configuration leading to melting.

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