Homogeneous melting of hard sphere crystals around its superheat limit

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A perfect crystal can be heated above its melting point when surface melting is avoided. This superheated crystal is metastable and melts through the nucleation of liquid phase. As getting higher above its melting point, the crystal becomes less metastable and finally reaches its superheat limit through a crystal instability. Here we identify that the superheat limit of hard sphere fcc crystal is set by Born's lattice instability that shear modulus vanishes, which is estimated to be at volume fraction about 0.493. Near the superheat limit, the liquid nuclei are triggered by particles moving in a chain while keeping the local crystal structure. In contrast to crystallization process that is commonly observed to be multi-stage, we show that melting is a single-step process by monitoring the evolution of the local order parameters of each particle.