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Observation of phase transitions in shocked Tin by molecular dynamics

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In classical shock theory, a phase transition leads to more or less marked discontinuities of the Hugoniot curve and can cause the split of the shock front. These characteristics are easily detected by the usual shock experiments, but the measurements are only indirect observations of phase transitions and give no information about the corresponding microscopic processes. Recent developments in new facilities (synchrotrons, free-electron X lasers) open up interesting new perspectives: the direct observation of the structural state behind the shock front becomes now possible. In parallel with these experiments, it is important to have proven simulation methods operating on the same scale as the basic phase transition processes, namely the microscopic scale. In this talk, we present a set of large-scale molecular dynamics simulations in a tin monocrystal, in which several phase transitions are expected under shock. The results are then compared with existing time resolved X-ray diffraction experiments.

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