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Ideal strength and structural instability of aluminum at finite temperatures[1] YI ZHANG, CHANGFENG CHEN, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, WEI ZHOU, HONG SUN, Department of Physics, Shanghai Jiao Tong University, China — Understanding the mechanical strength and stability of materials under different external conditions is of critical importance to material science and engineering. Despite of the extensive efforts on 0K ideal strength calculations in the past decade, the temperature effects on the ideal strength and dynamical stability have not been explored. We have calculated the ideal strength of aluminum at finite temperatures by implementing an ab initio molecular dynamics method (AIMD) that treats elastic instability, dynamic instability, and thermodynamics in a unified first-principles approach. The results reveal significant changes in fundamental mechanical properties of aluminum: (i) the ideal strength drops precipitously with increasing temperature, by as much as 60% at room temperature compared to T=0 K; (ii) the structural instability modes change qualitatively from dynamic phonon softening at low temperature to elastic failure at high temperature; (iii) the highly anisotropic low-temperature tensile strength becomes considerably more isotropic with rising temperature. Phonon calculations predict the disappearance of soft phonon modes near room temperature due to phonon anharmonic interactions, in excellent agreement with the AIMD results.

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Yi Zhang
Department of Physics and High Pressure Science and
Engineering Center, University of Nevada, Las Vegas

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