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Vibrational Properties of point defects and dislocations in metals BABAK SADIGH, Lawrence Livermore National Laboratory, PAUL SCHUCK, Arizona State University, VASILY BULATOV, Lawrence Livermore National Laboratory, WILHELM WOLFER, Lawrence Livermore National Laboratory — We calculate the vibrational spectra of vacancies, interestitials as well as dislocations in the fcc copper and bcc molybdenum described by interatomic potentials of the embedded-atom type. An in-depth study of the low-lying localized vibrational modes caused by the defects is presented. The concept of local atom-projected entropy within the harmonic approximation is introduced, and in this way the defect-indcued change in the thermodynamics of these metals is analyzed.

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