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Accuracy and applicability of the finite temperature quasicontinuum method LAURENT DUPUY, Lawrence Livermore National Laboratory, ELLAD B. TADMOR, Technion, Israel Institute of Technology, R. MILLER, Carleton University, ROB PHILLIPS, California Institute of Technology — The quasicontinuum method is a mixed continuum and atomistic approach for simulating the mechanical response of polycrystalline materials. It allows large-scale atomistic calculations to be performed on moderately small computers. This method was rencently extended to study the behavior of defects at finite temperature. In this talk, we focus on the accuracy and applicability of this method. Possible shortcomings such as mesh-dependence and ghost-forces are discussed.

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