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Analytical bond-order potential for aluminum

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Aluminum alloys are important structural materials because of their high strength-weight ratio, high thermal and electrical conductivities, high corrosion-resistance, and low cost. With very low hydrogen solubility, aluminum alloys have the potential for hydrogen-storage application without suffering from the hydrogen-embrittlement problem typical of steels. For this application, the long-time mechanical performance of the materials under hydrogen environment must be understood. Large-scale atomistic simulations based on interatomic potentials enable studies of the fundamental behavior of hydrogen with aluminum (e.g., adsorption, absorption, diffusion) as well as the interactions between hydrogen and crystalline defects such as dislocations. These studies can guide constitutive models to accurately predict material deformation over long-time scales. Numerous aluminum interatomic potentials exist, but none capture energy and geometry trends of different phases, making them problematic for studying defects (e.g., dislocations, hydrogen segregation, etc). Furthermore, we have found that angular-independent potentials have difficulty capturing both elastic properties and the high stacking fault energy characteristic of aluminum's face-centered-cubic (fcc) phase. Many literature angular-dependent potentials also poorly reproduce stacking fault energy due to inadequate parameterizations. In this work, we have developed an analytical bond-order potential (BOP) for aluminum. We show that this aluminum potential is transferrable to a variety of local configurations including defects and surfaces. More importantly, it simultaneously captures the elastic properties and stacking fault energy of the fcc phase. We are currently expanding our BOP to include both copper and hydrogen in an attempt to study hydrogen effects on Al-Cu alloys.

Biography

Xiao Wang Zhou has completed his Ph.D. at the age of 34 years from Clemson University. He is now a principal member of technical staff at Sandia National Laboratories. He has published more than 100 papers in reputed journals. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. This work is supported by the NNSA/DOE Office of Nonproliferation Research and Development, Proliferation Detection Program, Advanced Materials Portfolio.

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