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“SEEING” ATOMS AND BONDS WITH A COMPUTER

Advances in atomic probe technology (such as atomic force microscopy) have made it feasible to achieve unprecedented images of atoms and subatomic features like covalent bonds. However, fundamental questions remain about interpreting these images, which can have a close correspondence to the atomic structure of a given specimen, but sometimes do not. This situation is compounded by the difficulty in simulating such images. Simulated images are important to interpret and understand the atomic probe measurements. In order to perform computational studies of the image measurements one must determine the interatomic forces as a function of the atomic probe height above the specimen. Such a determination is computationally intensive and few examples of simulated images exist. We propose new high performance algorithms to solve for the forces between the atomic probe and the specimen. Our approach allows us to replicate the measured images and resolve outstanding issues in their interpretation.

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