

FINAL ABSTRACT**CRADA Title: Materials Modeling****CRADA Number: LA94C10167**

The primary purpose of this Cooperative Research and Development Agreement (CRADA) between Los Alamos National Laboratory and Molecular Simulations, Inc. (formerly Biosym Technologies, Inc.) was to create a set of computer modeling tools called the Lattice Model System (LAMS) that would accelerate the development of new materials. This set of materials modeling codes would model the atomistic properties of oxides, metals, and semiconductors and would be used to calculate the properties of polycrystalline materials. These models would not only incorporate the atomistic details of actual materials but would also capture the structural complexity of the materials in terms of their grain structures, diffusion, grain growth, and deformation and fracture properties. Principal project tasks were the structuring of microstructure modeling and related methods in a form appropriate for commercial release, the development of user-oriented graphics interface and analysis software, and the optimization of the materials modeling codes to run on a massively parallel computer environment. The grain growth modeling module was in development when the collaborative project was prematurely terminated because of a funding shortfall. Thus, the complete set of materials modeling codes, the Lattice Model System, was not developed.

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