Interatomic Forces in Covalent Solids

A thesis presented

by

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Dedicated to my father,

Zdeněk Pavel Bažant

with love, respect and gratitude.

Abstract

One of the outstanding unsolved problems in the physics of materials is that of designing a transferable interatomic potential for covalently bonded solids, such as Si, Ge and C. In spite of intense efforts which have produced over thirty fitted potentials for the prototypical covalent solid, Si, realistic simulations are still problematic for important bulk phenomena such as plastic deformation, diffusion, crystallization and melting. In this thesis, innovative analytic techniques are used to extract concrete information regarding the functional form of interatomic potentials directly from *ab initio* energy calculations. By deriving elastic constant relations we study forces mediated by sp^3 and sp^2 hybrid covalent bonds, and by inversion of cohesive energy curves we explore the covalent to metallic transition and angular forces. This body of results provides a reliable foundation upon which to build empirical potentials and develop our intuition about chemical bonding. These theoretical predictions can be captured using a new functional form with only a few adjustable parameters called the Environment-Dependent Interatomic Potential (EDIP). Efforts to fit an EDIP for Si have already led to unprecedented transferability for bulk defects. Work in extending the model to disordered bulk phases (liquid and amorphous) is underway, and extensions to related materials should be possible. The speed of force evaluation with the new model is comparable to the most efficient existing potentials, making possible large-scale atomistic simulations of covalently bonded materials with heightened realism.

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Citations to Previously Published Work

Portions of Chapters 3–5 have appeared (or will soon appear) in the following published articles:

Chapters 3 and 5 :	"Environment-Dependent Interatomic Potential for Bulk Silicon," M. Z. Bazant, E. Kaxiras and J. F. Justo, to appear in Phys. Rev. B (1997).
Chapter 4:	"Derivation of Interatomic Potentials by Inversion of *Ab Initio* Cohesive Energy Curves," M. Z. Bazant and E. Kaxiras, in *Materials Theory, Simulations and Parallel Algorithms*, ed. by E. Kaxiras, J. Joannopoulos, P. Vashista, and R. Kalia, Materials Research Society Symposia Proceedings Vol. **408** (Materials Research Society, Pittsburgh, 1996), p. 79.
	"Modeling of Covalent Bonding in Solids by Inversion of Cohehsive Energy Curves," M. Z. Bazant and E. Kaxiras, Phys. Rev. Lett. **77**, 4370 (1996).
Chapter 5:	"Interatomic Potential for Condensed Phases and and Bulk Defects in Silicon," J. F. Justo, M. Z. Bazant, E. Kaxiras, V. V. Bulatov and S. Yip, Materials Research Society Proceedings, Spring Meeting Symposium E (Materials Research Society, Pittsburgh, 1997).