# Atomistic Modeling of Semiconductors: Si, C, and 3C-SiC

An ongoing task of the Computational Materials Group (CMG) at the NASA Glenn Research Center is to enhance the role of atomistic simulations based on quantum-approximate methods in the study of new materials and their properties. One of the main goals of the activity continues to be breaching limitations that arise from the natural balance between accuracy, range of application, and computational simplicity (ref. 1). Whether that balance can be maintained while breaking new ground depends on the methods available with a minimum of constraints and limitations for the study of the energetics of arbitrary systems. The main tool used in CMG research, the Bozzolo-Ferrante-Smith (BFS) method for alloys (ref.2), has no inherent constraint in its formulation, a feature that has allowed for successful research on various topics. In this article, we report on the latest development of the CMG program, namely, the extension and application of the BFS method to compound semiconductors, a departure from our previous research based primarily on metallic alloys.

In spite of the differences between metallic systems and semiconductors, the straightforward formulation of BFS, which is based on a novel interpretation of the alloy formation process, remains unaltered, thereby providing an incisive predictive tool that is both physically sound and computationally simple. However, the particular nature of the elemental semiconductors Si and C and of the different silicon carbide (SiC) polytypes imposes a severe test of the method's accuracy because of radical differences in semiconductor and metallic bonding and because of the way such features are represented in the method.

The BFS energy calculations involve three pure element properties for each species: cohesive energy, lattice parameter, and bulk modulus. Two additional BFS perturbative parameters are determined from any pair of alloy properties. First-principles calculations using the self-consistent full-potential linearized-augmented plane wave (LAPW) method within the Generalized Gradient Correction as implemented in the WIEN97 program package (ref.3) were used to provide the three pure element properties for Si and C, as well as the equilibrium lattice parameter and zero-temperature energy of formation of 3C-SiC, to determine the perturbative BFS parameters for Si-C.
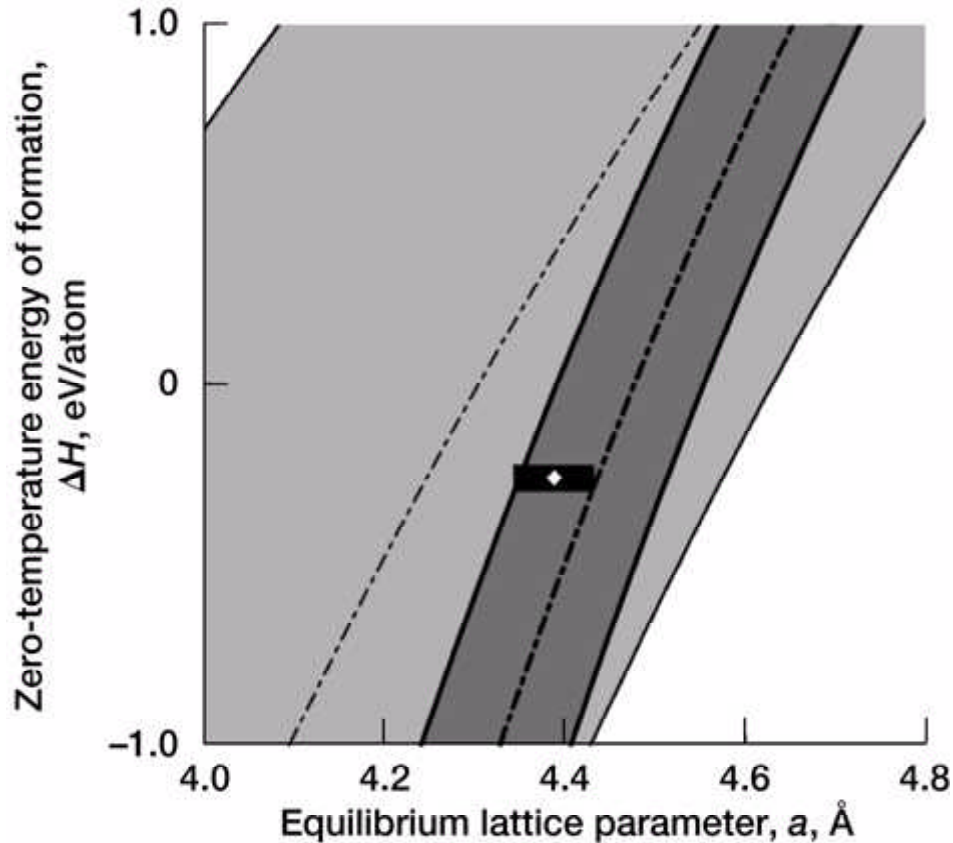
Region of validity of the BFS method: any input point (of equilibrium lattice parameter, a_0; and zero-temperature energy of formation, $\mathrm{D}H_0$) corresponding to the shaded region ensures the determination of transferable BFS parameters. The boundaries for Si- and C-valid regions (dark and light gray shade, respectively) are given by those points where the BFS contributions to the total energy of formation are bounded by the individual cohesive energy of the individual elements, Si and C (thick and thin solid lines, respectively).

The resulting parameters were compared with experimentally determined values where available. Once validated, these parameters will be fully transferable and applicable to any problem dealing with the SiC structure. First-principles calculations are usually accurate in predicting the value of equilibrium lattice parameters, but not as accurate in their prediction of the compressibility or the cohesive energy. These uncertainties necessarily translate into possible instabilities in the determination of the BFS perturbative parameters which should be such that the chemical energies associated with the equilibrium structure used as input (in this case, 3C-SiC) do not exceed their limiting values given by the cohesive energy of each type of atom. The preceding graph shows the regions where the BFS method is valid (i.e., if the LAPW-based point is located within the bands shown, then there is a guaranteed convergent solution to the BFS equations). The dashed curves (thick for Si, thin for C) trace the locus in the plane where the respective BFS chemical energies are zero, and the solid lines, above and below, indicate the points where the chemical energies reach their maximum allowed value.

The graph also shows a box surrounding the original LAPW point, defined as the region in the plane for which the equilibrium lattice parameter varies by 1 percent and the energy per atom varies by 10 percent, typical uncertainties in ab initio calculations. The fact that the uncertainty box is well within a unique region of the diagram ensures the validity of the LAPW input. The applications include the determination of the surface energy and structure of Si, C, Si-terminated (Si_t), and C-terminated (C_t) SiC (100) surfaces. Atomistic analysis of the formation of Si or C dimers on Si(100), C(100), and SiC(100) was also performed.

Numerous reconstruction models, backed by experiment, have been suggested to describe each of the Si(100) and Si_t or C_t 3C-SiC(100) surfaces. There are, however, conflicting and poorly understood features, as well as lack of consensus among the different theoretical techniques used to study what are, obviously, very complex systems. BFS predictions were compared with available experiment and other theoretical methods. The predicted values for dimer lengths and dimer/surface distance are in good agreement with experimental results in all the possible dimer/surface combinations (Si/Si, Si/C, Si/SiC, etc.). Dimer reconstruction of Si(100), as shown in the sketch, is one of the most studied features and, besides its numerous applications, it is a severe test for theoretical methods. The BFS values for the dimer length and spacing, in all cases, are well within the accepted range, raising confidence on the ability of BFS to reproduce the essential features of these systems.
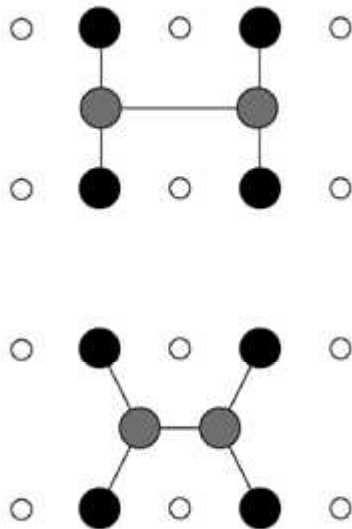
Rigid (top) and contracted (bottom) A-A dimer (A = Si, C) on a B(100) surface (B = Si, C, Si_t, or C_t 3C-SiC surface). Solid dark and light disks denote atoms in the surface and overlayer, respectively. Small circles denote atoms in the layer below the surface.

References

1. Bozzolo, Guillermo H., et al.: Software Package Completed for Alloy Design at the Atomic Level. Research & Technology 2000, NASA/TM-2001-210605, 2001,

pp. 16-17.

2. Bozzolo, G., et al.: Surface Segregation in Multicomponent Systems: Modeling of Surface Alloys and Alloy Surfaces. Comput. Mater. Sci., vol. 15, no. 2, 1999, pp. 169-195.

3. Blaha, P.; Schwarz, K.; and Sorantin, P.: Full-Potential, Linearized Augmented Plane-Wave Programs for Crystalline Systems. Comp. Phys. Comm., vol. 59, no. 2, 1990, pp. 399-415.

Find out more about this research:
Atomistic Modeling of Bulk Alloys, Surfaces and Interfaces
http://www.grc.nasa.gov/WWW/SurfSci/bfs/bfs_index.html
Tribology & Surface Science Branch http://www.grc.nasa.gov/WWW/SurfSci/

OAI contact: Dr. Guillermo Bozzolo, 440-962-3103, Guillermo.H.Bozzolo@grc.nasa.gov
Glenn contact: Dr. Phillip B. Abel, 216-433-6063, Phillip.B.Abel@grc.nasa.gov
Authors: Dr. Guillermo Bozzolo, Dr. Jorge E. Garces, and Dr. Phillip B. Abel
Headquarters program office: OAT
Programs/Projects: HOTPC