

## Errata

### Erratum: Atomic structure and ordering in semiconductor alloys [Phys. Rev. B 31, 2561 (1985)]

G. P. Srivastava, José Luís Martins, and Alex Zunger

In our paper we calculated the total excess energy  $\Delta E^{(n)}$  of ternary  $\text{Ga}_n\text{In}_{4-n}\text{P}_4$  ordered phases ( $n=1,2,3$ ) relative to equivalent amounts of the constituent binary solids GaP ( $n=4$ ) and InP ( $n=0$ ), finding  $\Delta E^{(2)} = -1.38$  kcal/mol for the CuAu-*I*-like  $\text{GaInP}_2$  structure. This calculation used a nonrelativistic *local* pseudopotential, obtained by averaging and smoothing the “hard core” *s* and *p* atomic pseudopotentials. It underestimated the observed (0.42 Å) lattice constant mismatch  $a(\text{InP})-a(\text{GaP})$  by 0.2 Å, hence<sup>1</sup> also  $\Delta E^{(2)}$ . Correcting for this effect alone produced<sup>1</sup>  $\Delta E^{(2)} = -0.29$  kcal/mol (−25.2 meV per 4-atom formula unit); the chalcopyrite structure was found to be 0.1 kcal/mol more stable.

We repeated the calculation for  $\text{GaInP}_2$  in both the chalcopyrite and the CuAu-*I* structures using the semirelativistic all-electron (linear-augmented-plane-wave) (LAPW) method.<sup>2</sup> For the binaries, we find  $a_{\text{InP}} = 5.918$  Å (expt: 5.866 Å),  $a_{\text{GaP}} = 5.462$  Å (expt: 5.450 Å). For the CuAu-*I* structure, we find  $\Delta E^{(2)} = +91$  meV/4 atoms (+1.05 kcal/mol), rather than our corrected pseudopotential value of −25.2 meV, whereas for chalcopyrite, we find  $\Delta E^{(2)} = 19$  meV/4 atoms (+0.22 kcal/mol).

Our corrected result for  $\text{GaInP}_2$  in the CuAu-*I* structure is close to the value of 83.6 meV/4 atoms obtained by Boguslawski and Baldereschi<sup>3</sup> for  $\text{GaInAs}_2$ . The new positive excess energy obtained here shows that the predicted  $\text{GaInP}_2$  ordering is *metastable*, as illustrated in Ref. 1 (i.e., the ordered phase has a lower energy than the disordered phase, but higher than the GaP-InP phase-separated system), rather than *stable* ordering (the ordered phase having a lower energy relative to both the disordered and the phase-separated system) as we claimed earlier.

<sup>1</sup>A. A. Mbaye, L. G. Ferreira, and A. Zunger, Phys. Rev. Lett. **58**, 49 (1987); A. A. Mbaye and A. Zunger, in *Ternary and Multinary Compounds*, edited by S. K. Deb and A. Zunger (Material Research Society, Pittsburgh, PA, 1987), p. 365.

<sup>2</sup>S.-H. Wei and H. Krakauer, Phys. Rev. Lett. **55**, 1200 (1985).

<sup>3</sup>P. Boguslawski and A. Baldereschi, Solid State Commun. **66**, 679 (1988).

### Erratum: Long-range order in $\text{Al}_x\text{Ga}_{1-x}\text{As}$ [Phys. Rev. B 36, 1526 (1987)]

J. S. Cohen and A. G. Schlijper

In a previous paper we reported on a self-consistent calculation in the local-density approximation of the ordering energies of  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  alloys with the use of the augmented-spherical-wave (ASW) approximation. These results appear to be at variance with the results that have been obtained by various other authors using a pseudopotential method<sup>1</sup> and the augmented-plane-wave method.<sup>2</sup> We have investigated this problem and we find that the results are very sensitive to the choice of empty spheres that are needed to handle the interstitial regions, which are large in the zinc-blende structures.

In the ASW calculations as performed earlier, two different species of empty spheres were used. One type of empty sphere ( $Z_0^{\text{As}}$ ) was placed in the interstitial sites in the planes containing only As atoms. The other type ( $Z_0^{\text{Al}}$ ) was used in the planes containing Al and Ga atoms. Both species of empty spheres were given the same radius, but were allowed to contain a different density of electrons. This choice of empty spheres imposes a symmetry between the Al planes and the Ga planes. The atomic radii were chosen such that for each element a fcc crystal has zero pressure. This set of parameters is denoted *A* in Table I. The lattice constant is denoted by *a*. Parameter set *A* is not correct at two points; it