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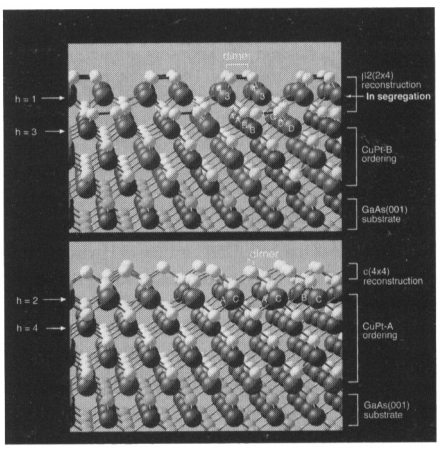
COMPOSITIONAL MODULATION AND ORDERING IN SEMICONDUCTORS

MRS NEWS

ABSTRACTS

DEPARTMENTS



ON THE COVER: These figures show the predicted lowest energy configurations of a (100) film of $Ga_{0.5}In_{0.5}P$ (Ga = blue, In = red, P = yellow) on a GaAs(100) substrate (As = green), illustrating the relation between (a) surface reconstruction, (b) surface segregation, and (c) subsurface ordering. TOP: When the reconstruction is β2(2 x 4), In segregation (red atoms under the dimers) and CuPt-B ordering (alternating <111> planes of In and Ga) exist. CuPt-B ordering implies that there is Ga under the dimer (site A) and In between dimer rows (site C). If we swap these Ga and In atoms, a large strain field results, raising the total energy by 150 meV/pair. This shows that the CuPt-B arrangement is stable. BOTTOM: When the reconstruction is c(4 x 4) with the surface dimer rotated by 90° with respect to those of β2(2 x 4), the In segregation disappears and the subsurface ordering changes from CuPt-B to CuPt-A. In this case, we have Ga occupying sites A and B, while In occupies site C. Ordering leads to major changes in material properties, including bandgaps, polarization, band offsets, and internal electric fields. For more details on these calculations, see the following: S.B. Zhang, S. Froyen, and A. Zunger, *Appl. Phys. Lett.* **67** (1995) p. 3141; S. Froyen and A. Zunger, *Phys. Rev. B* **53** (1996) p. 4570; and "Spontaneous Atomic Ordering in Semiconductor Alloys: Causes, Carriers, and Consequences," by A. Zunger on page 20 of this issue.

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Materials Research Society
9800 McKnight Road
Pittsburgh, PA 15237-6006
Tel. (412) 367-3003; Fax (412) 367-4373
http://www.mrs.org/

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Editorial Office • 9800 McKnight Road • Pittsburgh, PA 15237-6006
Tel. (412) 367-3004 x522; fax (412) 367-4373; http://www.mrs.org/

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Associate Editor—Europe
I.W. Boyd, University College London
Dept. of Electronic and Electrical Engineering
Torrington Place
London WC1 E7 JE, U.K.
Tel. 44-171-380-7300 or 7302

Book Review Editor
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MRS Office of Public Affairs
601 13th Street, NW, Suite 1000 South
Washington, DC 20005-3807
Tel. 202-661-2285, Fax 202-661-2299

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