**SESSION C23: SEMICONDUCTION I: SUPERLATTICES**
**Monday afternoon, 12 March 1990; Palos Verdes Room at 14:30; A. Jones, presiding**

*Invited Paper*

**14:30**

**C23 Stability of Semiconductor Superlattices and Their Alloys.'** ALEX ZUNGER. ***Solar Energy Research Institute***

Most theoretical research on semiconductor superlattices focused on their electronic properties. Here I will discuss the thermodynamic stability [I] of **a variety** of strained-layer superlattices [CaAs-GaSb, GAP-GaAs, CaP-InP, GaAs-InAs, AlP-InP, ZnTe-HgTe and ZnTe-CdTe]in different **orientations**. Artificial growth of ApBp superlattices (SL's) is based **on a series** of sequential **exposures of a substrate to** the pure compound A then **pure B,** etc., thus largely circumventing the thermodynamically controlled simultaneous reaction $xA+(1-x)B \rightarrow A_xB_{1-x}(\gamma)$ **which** could have produced a variety of structures y ranging from disordered alloys to phase separation. Rather than focus on simulation of **growth kinetics,** I ask here how stable is an already grown SL **with** respect to decomposition into its constituents or to disordering into **an** alloy and how does the repeat period p and orientation $\xi$ affect the above. These questions are addressed by (i) first-principles (LAPW and psuedopotential) calculations of the total energies of ordered $A_pB_p$ SL's, and (ii) statistical mechanics (cluster-variation) calculations for the disordered $A_{0.5}B_{0.5}$ alloys (21. This shows: (i) the dominance of strain over charge transfer **iffectr** leads to the instability of all bult SL's with respect to **disproportionation, except** (ii) $(AlX)_2(InX)_2$ for X=P, and As where the opposite ***is* true in the chalcopyrite structure. (iii)** The stability order. **for Long p→∞ bulk SL's** is **[001]>[201]>[110]>[111], reflecting the sequence of** the biaxial strain in the binaries. (iv) For small p's, there are "magic numbers" whereby **p=2[110]** and **[201] SL's** are the atablest, owing to an effective interfacial **relaxation (v) the 50%-50% random** alloy is stabler than **all SL's except those at the** "magic numbers", for which **spontaneous Long range** ordering of an alloy **is** possible, (vi) **the** stability of epitaxial **SL's** on a lattice matched substrate is greatly enhanced **relative to bulk** due to the destabilization **of the** decomposition products.

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[1] R. C. Dandrea, J. **E.Bernard,** S.-B. **Wei** and A. **Zunger,** submitted to **Phys.** Rev. Letters.
[2] L. C. **Ferreira, S.-H. Wei** and A. Zunger, **Phys.** Rev. **B40, 3197(1989).**