Extended Abstracts of the 20th (1988 International) Conference on Solid State Devices and Materials, Tokyo, 1988, pp. 625-626

LC-5-3

Comprehensive Analysis of Lattice Strain in Heteroepitaxial Layers

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In this paper, we propose a comprehensive model for the lattice strain in heteroepitaxial layers and discuss the effect of the lattice strain on the energy band structure.

There are two dominant causes for the lattice strain in heteroepitaxial layers. One is the lattice misfit stress and the other is the thermal stress. When the thickness of the layer is sufficiently thin, the in-plane lattice constant of the epilayer matches that of the substrate at the heterointerface. Therefore, the lattice misfit is accomodated by elastic lattice strain in epilayers. As the thickness increases above the critical thickness for generation of misfit dislocations, the misfit stress is relieved. Then, the themal stress dominates eventually in thick epilayers.

We have calculated residual stress in heteroepitaxial layers based on the model mentioned above, using the Mathews model for the misfit stress and the bimetallic strip model for the thermal stress. Dependences of the residual strain in heteroepitaxial layers on the layer thickness are classified into four cases depending on the relations of lattice parameter and thermal expansion coefficients between the substrate and the epilayer: (1) $a_e > a_s$ and $\alpha_e > \alpha_s$; (2) $a_e > a_s$ and $\alpha_e < \alpha_s$; (3) $a_e < a_s$ and $\alpha_e > \alpha_s$; (4) $a_e < a_s$ and $\alpha_e < \alpha_s$. The calculated results are schematically shown in Fig. 1. In the case of (1), the misfit stress is biaxially compressive, although the thermal stress is biaxially tensile. There is a coherent biaxial compressive strain in the layers thinner than the critical thickness, while a biaxial tensile strain dominates in the layers much thicker than the critical thickness. The calculated residual strain is compared with experimental results of various heteroepitaxial systems including GaAs on Si, InGaAs on GaAs, SiGe on Si, and ZnSe on GaAs. Fair agreements are obtained except around the critical thickness.

We have calculated the splitting of the valence band and shifts of the energy bandgap as a function of layer thickness. We have found again fair agreements between the experimental results and the calculation except around the critical thickness.

In conclusion, we have proposed a model for the lattice strain in heteroepitaxial layers based on the idea that the misfit and thermal stresses are dominant causes for residual lattice strain. Calculated dependences of residual strain and shifts in energy bandgap are in fair agreements with experiment results.

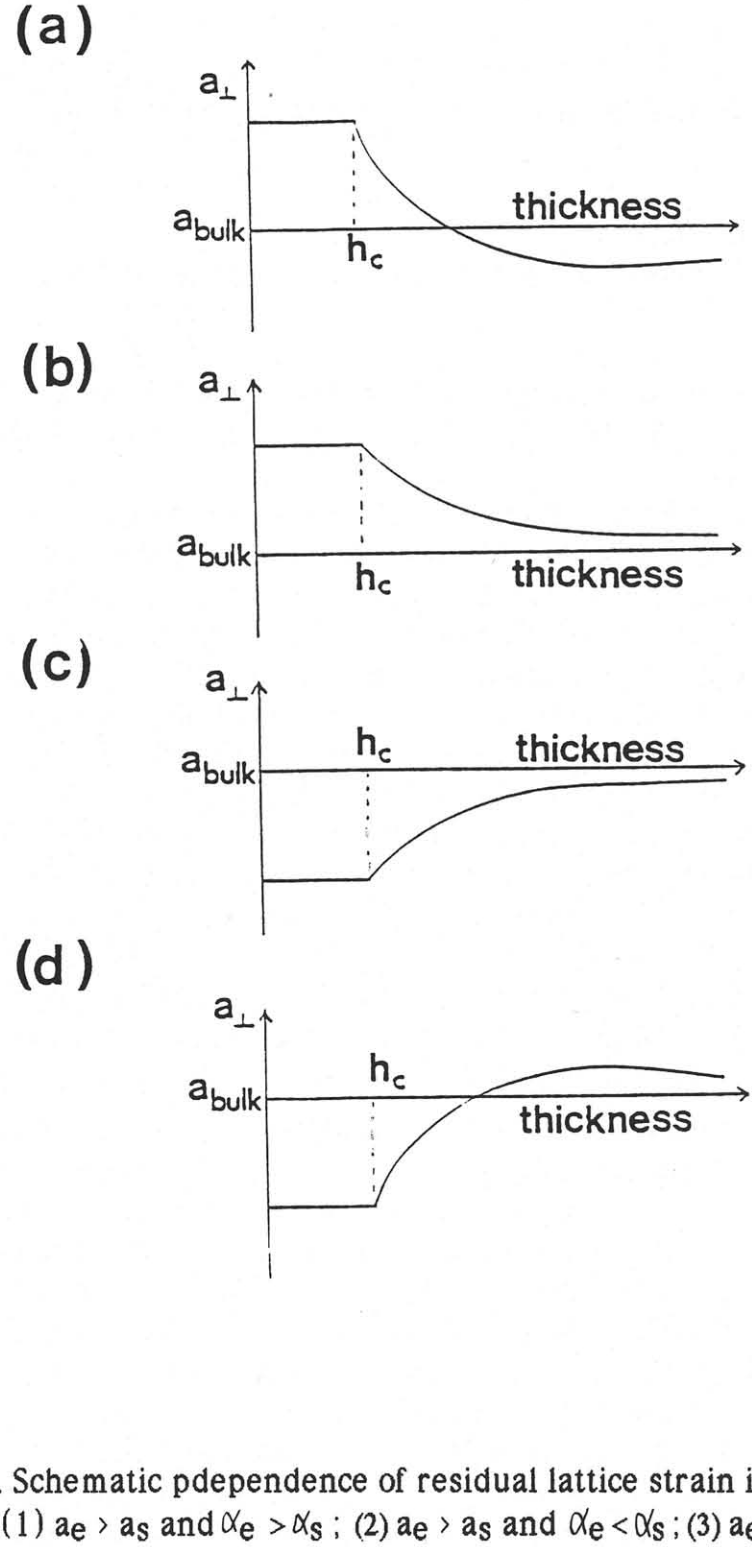

Figure 1. Schematic pdependence of residual lattice strain in heteroeppitaxial layers. (1) $a_e > a_s$ and $\alpha_e > \alpha_s$; (2) $a_e > a_s$ and $\alpha_e < \alpha_s$; (3) $a_e < a_s$ and $\alpha_e > \alpha_s$; (4) $a_e < a_s$ and $\alpha_e < \alpha_s$.