PHILOSOPHICAL MAGAZINE A, 1995, VOL. 72, NO. 6, 1531–1545

TS124

A model for the distribution of misfit dislocations near epitaxial layer interfaces

By G. MACPHERSON, P. J. GOODHEW and R. BEANLAND

Department of Materials Science and Engineering, University of Liverpool, Liverpool L69 3BX, UK

[*Received 6 December 1994 and accepted 9 May 1995*]

ABSTRACT

We present Monte Carlo simulations of the process of misfit relief in strained epitaxial layer interfaces. The emphasis is on the effect on the distribution of dislocation spacings owing to the reactions of 60° dislocations to form edge dislocations. When there are no edge dislocations the distribution is a decaying exponential function, but as the edge dislocation density increases a peak appears in the distribution. The position and magnitude of this peak depend on the proportion of edge dislocations found within the misfit dislocation array. We also take into account the effects of the experimental resolution on the appearance of the histograms. The results are consistent with detailed experimental measurements of dislocation spacing distributions and are important since the energy of an array increases significantly when the dislocation spacings are non-periodic.

§ 1. INTRODUCTION

Pseudomorphic heteroepitaxial layers are generally strained with respect to their substrate because of the differences between lattice parameters. Most of the elastic strain in a layer can be relaxed if misfit dislocations (MDs) are introduced at the interface. Such misfit dislocations must have a component of their Burgers vector in the plane of the interface, but the exact nature of the dislocations is usually controlled by the availability of mechanisms for introducing them, rather than by the deepest minimum in the energy of the system.

It is well established that there is a critical thickness above which it is energetically favourable for MDs to be present. Many models for the critical thickness have been published (Frank and van der Merwe 1949, Matthews and Blakeslee 1974, People and Bean 1985, 1986) and there is substantial experimental evidence that dislocations appear in most strained epitaxial systems after the Matthews and Blakeslee critical thickness (h_c) has been exceeded (Matthews and Blakeslee 1974). It is also clear that strained layers rarely, if ever, relax completely, that is, so that the content of MDs at the interface is sufficient to reduce the strain in the epilayer to zero. Strain relaxation processes often continue until the layer thickness is well in excess of the critical value h_c. There are many reports of layers 100 times thicker than h_c which are still significantly strained (Dunstan *et al.* 1993).

Arrays of MDs rarely show a regular spacing (Abrahams, Blanc and Buiocchi 1972, Noble *et al.* 1990), and in the early stages of relaxation of (001) semiconductor layers the two orthogonal sets of MDs may not even have the same mean spacing (Matthews and Blackslee 1974). The distribution of spacings has not been studied quantitatively until recently (MacPherson *et al.* 1994), although it is known that