Atomic structure of twist bonded interfaces: a molecular dynamics study

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Wafer bonding, i.e. creating interfaces by joining two wafer surfaces, is already widely applied in microelectronics, micromechanics or optoelectronics. The macroscopic properties of bonded materials, however, are strongly influenced by the atomic processes at the interfaces during the transition from adhesion to chemical bonding. Thus, the description of the atomic processes is of increasing interest to predict the bonding behavior. Molecular dynamics simulations using empirical potentials (cf., e.g., [1]) have been performed to describe atomic interactions at interfaces, enabling to study the processes with macroscopic relevance.

Whereas bonding of two perfectly aligned wafers give a single, perfectly bonded wafer without defects, miscut of the wafer results in steps on the wafer surfaces and thus edge dislocations at the bonded interfaces. Bonding wafers with rotational twist leads additionally to a network of screw dislocations (cf., e.g., [2,3]). The present paper investigates the bonding processes as a function of the twist angle, thickness of the wafers, and annealing temperature.

The effect of a small twist angle as a rotational misorientation results in a mosaic-like interface structure [4]. Fig. 1 shows some of the resulting minimum structures gained for higher annealing temperatures and different twist rotation angles. Before the bonding process takes place, the superposition of the two wafers looks like a Moiré pattern in the projection normal to the interface. After bonding and sufficient relaxation under slow heat transfer conditions, almost all atoms have a bulk-like environment separated by misfit screw dislocations, which may have a high rate of kinks. The screw dislocation network of the bonded wafer has a period half of those of the Moiré pattern. One reveals the more located imperfectly bonded regions around the screw dislocations for smaller twist angles, whereas bonding at higher angles result in more or less widely spread strained interface regions. Whereas simulations with parallel dimerization and larger angles at start clearly demonstrate the creation of the screw dislocation network, for orthogonal dimerization or small twist angles this is no longer valid. The periodicity of the defect region is twice of those of the examples shown in Fig. 1 smoothing out the interface, but creating additional shear strains. Varying slightly with the twist angle the final structures yield bond energies of approximately $4.5 eV/atom$ at $0K$ with a maximum occuring between 4° and 6° twist. As higher the annealing temperature as better the screw formation.

Thus the misalignment due to twist rotation of the wafers influences the bondability of larger areas, and different defect and atomic arrangements at the interfaces occur. In addition, if very thin wafers are being bonded the free surfaces are modified by the resulting interface relaxation. Unlike bonding bulk wafers, the MD simulations for thin wafers yield effects at the free surfaces, like welding and straining, not compensated also in DFT-LDA simulations [5]. Modifications of the band structure due to different interface relaxation occur which may enable tailoring of the electronic properties. The simulations lead to a better understanding of the physical processes at the interfaces and support the experimental investigations, especially the electron microscope structure analysis.

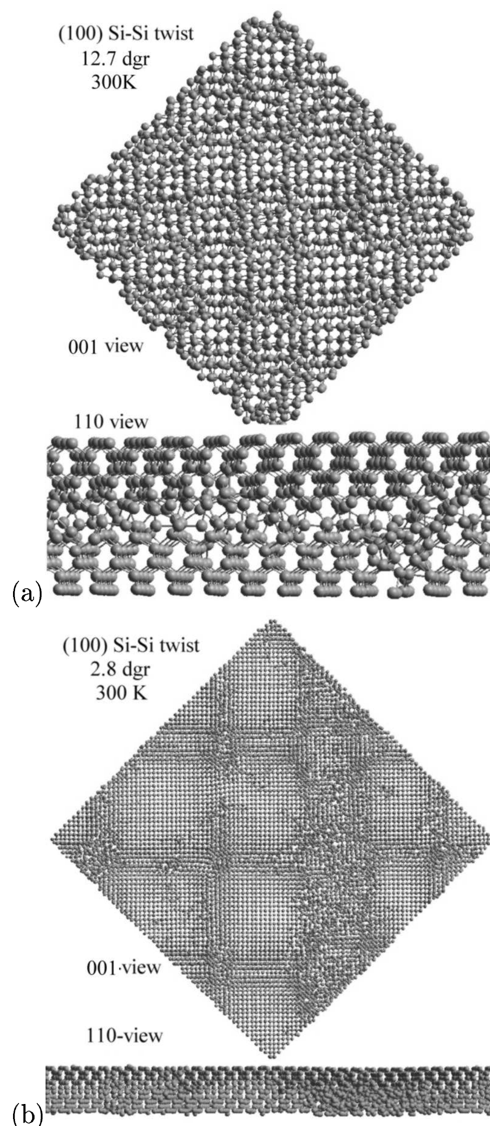

Figure 1

MD simulated structural models ([001] and [110] views) of bonded wafers with different rotationally twist angles annealed at 300K for parallel dimer start configurations: (a) 12.7°, 6500 atoms, 4.9nm box; (b) 2.8°, 134500 atoms, 22nm box, and with additional bonding over steps.

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