Bonded Semiconductor Interfaces with Twist and Tilt Rotation: TEM Analysis supported by Molecular Dynamics Structure Modelling

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Hydrophobic Si wafer direct bonding with controlled rotational misalignment is a promising approach for the formation of self-organised patterns of geometrically defined biomolecular complexes on silicon surfaces [1]. The rotational (twist) misalignment creates a square network of screw dislocations at the bonded interface whereas the inevitable miscut (tilt) of the wafers causes bonding over steps. The atomistic processes during the transition from the adhesion state to the chemical bonding strongly determine the special defect configurations at and properties of the bonded interfaces.
Transmission electron microscopy (TEM) has been applied to investigate the bonded interfaces at an atomic level. Molecular dynamics (MD) simulations have been performed to study atomic processes related to the reordering at interfaces and relaxation of nanostructures [2]. To enhance MD, a bond order potential based on an analytic tight binding approximation is used in addition to the empirical Tersoff potential. It allows calculations of macroscopically relevant systems preserving the essential quantum mechanical nature of atomic bonding, yet abandons the electronic degree of freedom. The implementation of BOP4 is based on [3] but includes a number of angular terms ignored previously describing certain bonds between neighbouring atoms. The MD relaxed structures are the basis for enhancing the TEM image analysis.
In addition to former investigations of twist misalignment simulations to include the tilt effect of bonding are performed. Fig. 1 shows an experimental TEM image of a bonded interface with 1.5° twist and 0.53° tilt. Fig. 2 shows the MD relaxed structure of a bonded 100-Si interface with 6.7^{o} twist, i.e. the resulting screw dislocation network, and different typical TEM image simulations for varying bonding and imaging conditions.

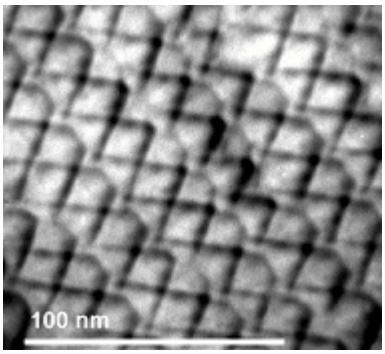

Fig. 1: Experimental 200 kV bright-field diffraction contrast at a bonded interface with 1.5° twist and 0.53° tilt

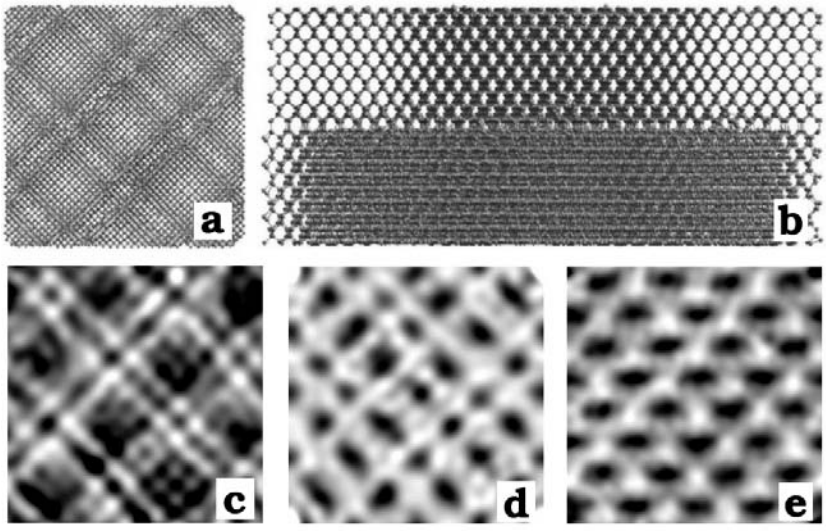

Fig. 2: MD relaxed structure model of a 6.7^{o} twist bonded interface in a) 001- and b) 110-view, and simulated TEM images (400kV, ca. 40nm thickness) with twist misalignment of c) 4.3^{o} d) 6.7^{o} e) 83.3^{o}.

References

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