Molecular dynamics simulations to investigate wafer bonded interfaces

Kurt Scheerschmidt [*], Detlef Conrad, Ulrich Gösele

Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany

Abstract

The physical processes of wafer bonding and the resulting structure of interfaces are studied by the combined use of molecular dynamics (MD) structure modelling and high resolution electron microscopy (HREM) structure imaging.

Keywords: Molecular dynamics; Wafer bonding; High resolution electron microscopic materials characterization

1. Introduction

Silicon wafer bonding has increasingly become promising for silicon-on-insulator and micromechanical applications. The bonding energy and forces strongly depend on the surface structure (native oxides, adsorbates, hydrophobic or hydrophilic termination) and the bonding control equipment (atmospheric or UHV bonding, annealing temperature and time). For a better understanding of the physical processes of wafer bonding the experimental investigations are supported by theoretical analyses of the interaction of the atoms at the surfaces contacting each other. The physical processes of wafer bonding and the resulting structure of interfaces are investigated by applying and combining high resolution electron microscopy (HREM) and molecular dynamics (MD) simulations. HREM is a routine technique of structural characterization of materials as it locally provides information at an atomic level. However, a direct interpretation of the electron micrographs is mostly not possible, because the HREM contrast depends strongly and nonlinearly on the imaging conditions and the scattering behavior of the structure investigated. Thus the interpretation of HREM micrographs requires image analysis and the computer simulation of the HREM contrast by calculating the electron beam/specimen interaction of a theoretical structure model and by subsequently considering the electron-optical process. MD simulations enable theoretical investigations to be made of atomic interactions, including structural relaxations and dynamic processes, and thus the simulation of resulting physical properties. Classical MD solves the equations of motion of an ensemble of particles assuming suitable interatomic potentials and boundary conditions.

2. Coherent interfaces

HREM imaging and MD modelling are applied and tested as to investigate multi-layer structures, quantum wells and quantum dots for binary and ternary compounds of semiconductors [1,2], silver particles in sodium–silicate glasses by relaxing dis-

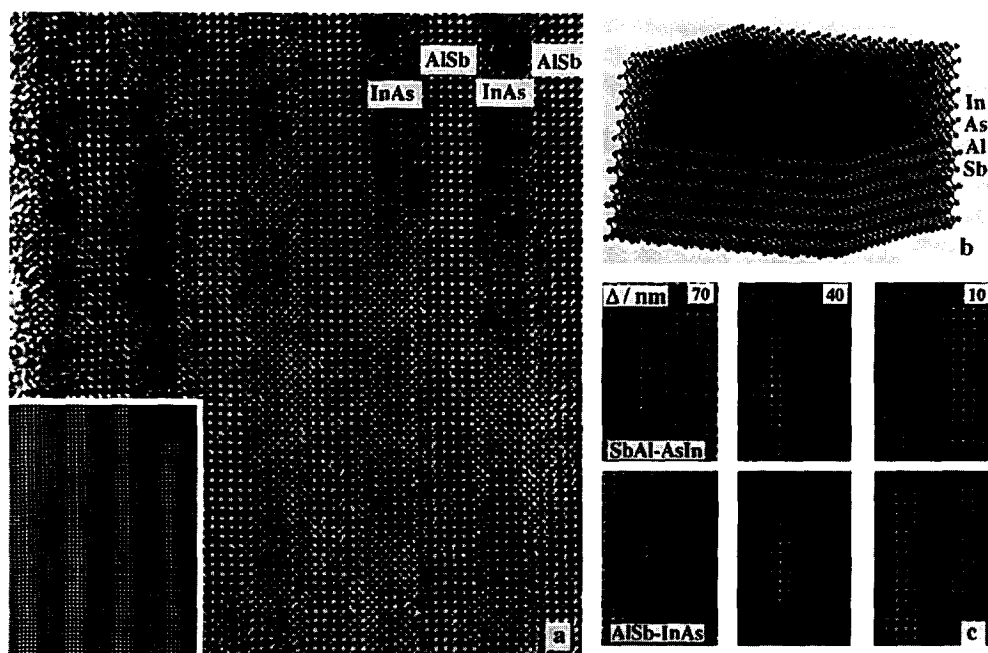* Corresponding author. Tel.: +49-345-5582910; fax: +49-345-5511223; e-mail: schee@mpi-msp-halle.mpg.de.

Fig. 1. (a) Experimental 400 kV HREM image of a (1.8 nm InAs/1.8 nm AlSb)$_n$ multi-layer structure and section filtered with {200} beams (insert); (b) MD relaxed structure model and (c) corresponding simulated images using different defoci Δ for 2 different atomic sequences across the interface. Imaging parameters: $U = 400$ kV, $C_s = 1$ mm, $\delta = 8$ nm, $\alpha = 0.5$ mrad, $t = 11.3$ nm.

turbed and topologically rearranged sodium silicate crystals after sodium–silver ion exchange [3], and grain boundaries in Au and Ge. As an example, in Fig. 1 the InAs/AlSb system is characterized by a large misfit and a remarkable structure factor asymmetry as well as by two most different interfaces: InSb having a small asymmetry, AlAs having a large one. Fig. 1a shows a HREM micrograph of the InAs/AlSb multi-layer system and its contrast enhancement by Fourier filtering of the {200} reflexions (inset). The analysis reveals the layer sequence (InSb and AlAs interface) and to identify the roughness of the interfaces (steps). The interfaces are no longer abrupt. Local variations of the orientation, however, create virtual boundary structures, which cannot be analyzed in a phenomenological manner. In some places finer fringes occur, which can be interpreted as 'half spacings'. Such features are less pronounced in the experimental images than in the simulated ones according to the relaxation, which was calculated by minimizing the energy of the structure including the misfit (Fig. 1b). The layers have the same crystallographic structure; heterostruc-

tures were generated by replacing atoms and changing the equilibrium distances. As the interfaces are assumed to be coherent, a relaxation by molecular statics using simple Morse potentials and Fourier-angular terms is supposed to yield reasonable results, explaining the strains at the interface and the resulting contrast. In the simulated defocus series of Fig. 1c, for underfocus values of 70, 40, and 10 nm, the strong contrast dependence on thickness, imaging orientation and sample preparation shown here, does not allow the unambiguous characterization of the interfaces themselves. Nevertheless, in most of the cases the different layers can clearly be distinguished and their atomic columns or pairs can directly be imaged. Varying the defocus may change the orientation of the striations according to the strains.

3. Wafer bonding

Mirror-polished and flat pieces of solids adhere to each other provided there are no dust particles between the surfaces. This is well known and holds
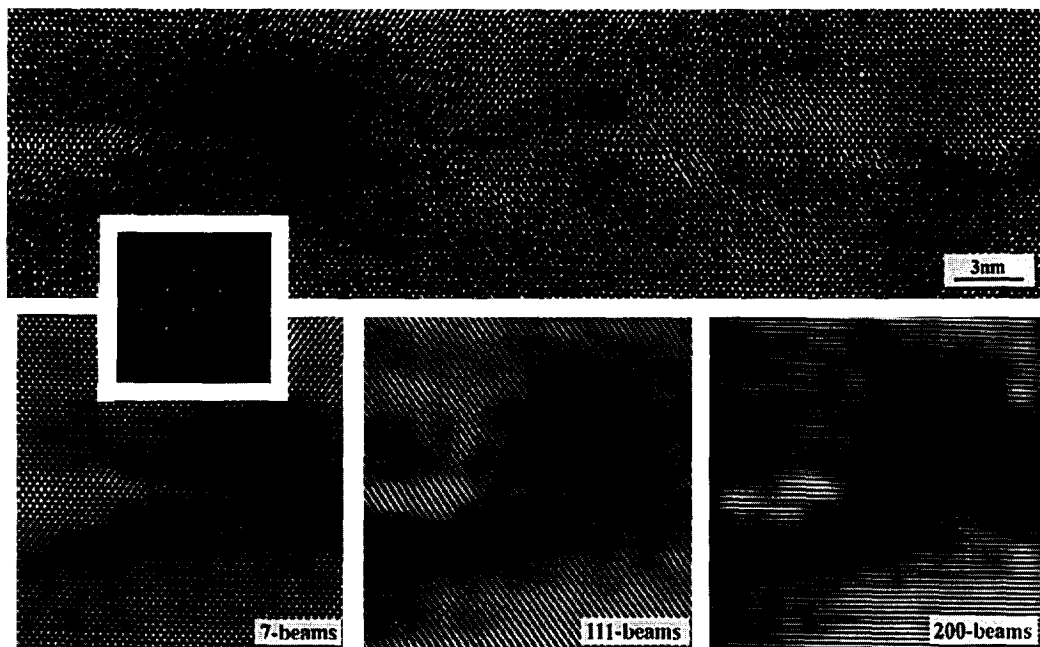
Fig. 2. UHV bonded Si(100)-wafers: 400 kV Si(110)-HREM, optical diffraction and filtered images.

good for a large number of materials, but the simplest experiments can be made using commercially available silicon wafers and a microclean room set-up: chemically prepared wafers are cleaned and dried by rotating and heating up the wafers. A slight attachment of the wafers starts the bonding, which may be controlled by infrared imaging. Both hydrophilic and hydrophobic wafer bonding imply rather weak bonding energies relative to those of covalent bonding. High bonding energies are attained by annealing the room temperature bonded wafers at high temperatures. For a number of applications it would be desirable to reach the bulk bonding strength by room temperature bonding with no additional heating step necessary. This was done for the first time: UHV experiments demonstrate that large area, self-propagating, room-temperature covalent wafer bonding of commercially available (100) silicon wafers is possible [4]. Removing the native oxide by hydrofluoric acid, rendering the surfaces hydrophobic and covered with hydrogen, made the wafer bonded as usual in a microclean room. In the UHV chamber the bonds were separated, hydrogen was removed by heating, pumping and cooling before

finally the room-temperature bonding started. Fig. 2 shows the resulting structure, viz. the example of an interface of room-temperature UHV-bonded silicon wafers investigated by cross-sectional HREM. Though not showing any noticeable intermediate layer the interface does not correspond to a perfect structure. This may be due to incomplete bonding processes arising from misorientations of the two wafers, fast energy dissipation, or defects remaining at surface structures as, e.g., at surface steps. The filtered images additionally show lattice planes indicating interfacial dislocations.

4. MD-simulations

The simulation of the bonding process for macroscopically relevant structures requires a large number of particles to be considered and many-body empirical potentials to be applied. In addition, the dynamics of this problem is much more complex than that for coherent boundaries. Probable changes of the structure and macroscopic thermoelastic boundary

conditions have to be included. In addition, two important considerations should be regarded to usual classic MD simulations [5]. The potential most often used for group IV semiconductors is the Stillinger–Weber potential. Originally proposed for silicon it consists of a two-body and a three-body part. The three-body part ensures that the diamond structure is the stablest of all. The parameters are fitted to the lattice constant, the cohesive energy, and the melting point of crystalline silicon. In the diamond structure the potential has a smooth cut-off behind the nearest neighbor distance scaling with respect to the cohesive energy and the nearest neighbor equilibrium distance. That means, if only these quantities are replaced by the quantities of another diamond-structure material, a reasonably good potential is obtained without fitting the whole set of parameters. Such rescaled potentials were used for studying the properties of germanium, diamond, germanium–silicon alloys, GaAs. The interactions of two silicon surfaces, however, can be studied by additionally revealing the 2×1 reconstruction of a clean Si(100) surface. While the Stillinger–Weber potential correctly predicts a lower energy for surfaces reconstructed relatively to those of the ideally truncated bulk, the dynamical behavior can only be achieved if the system is heated up to reduce the distance of the surface atoms. One may improve the Stillinger–Weber potential by adding new terms, but it is possible to enhance it qualitatively without changing the functional form. We use a second order parametrization of the Stillinger–Weber potential which was proposed for simulating the diamond (100) surface together with the length and energy scales for silicon. This new potential leads to the dimerization of the Si(001) surface within a few 100 fs. The energy gain of creating a dimer bond is 1.77 eV, which is in good agreement with ab initio results (1.92 eV).

The second improvement is related to the energy transfer, because even the deposition of single atoms may lead to the melting of the surface during the simulation, according to the fact that every new bond implies an energy gain of eV order, which is distributed in a constant energy simulation onto a small number of atoms. Therefore two approaches are applied to rescale the velocities of the outermost atomic layers, to either an average constant tempera-

ture, or with a constant reduction factor. It should be considered as a certain way of simulating macroscopic heat conduction, and hence, the flow of kinetic energy away from the interface. This temperature control was applied every 100 time steps, where the kinetic energy was averaged over the 100 time step intervals. A more frequent rescaling would affect the lattice vibrations. The first approach suggests a situation in which the heat conduction takes place very fast, therefore termed 'fast heat conductioi approach'. In the second approach the kinetic energy
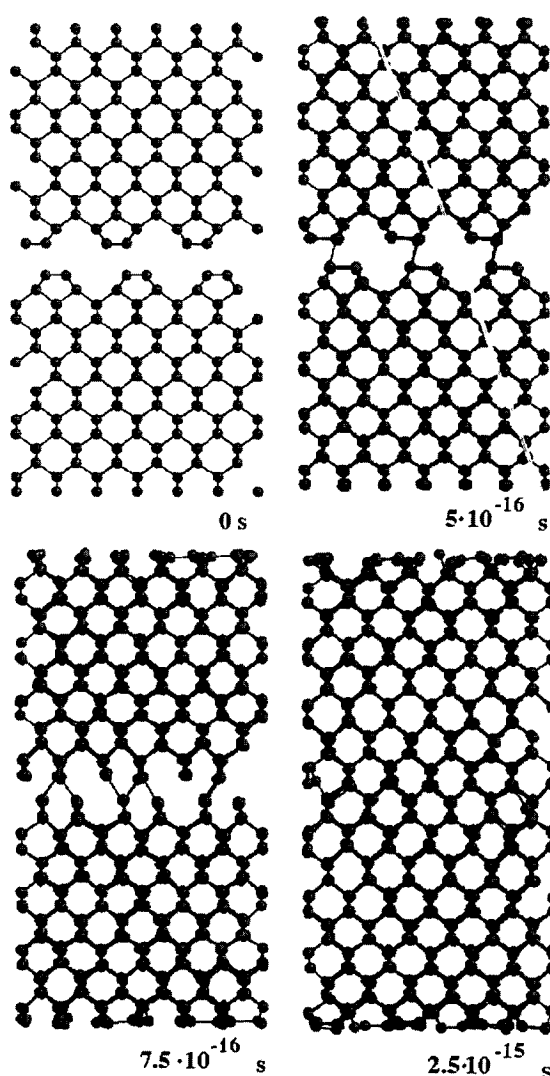

Fig. 3. Snapshots of MD simulated Si(100) wafer bonding: perfect alignment of the dimerized surfaces, slow heat conduction.

of the outermost atoms is scaled and averaged every 100 time steps by the constant factor of 0.98, termed 'slow heat conduction approach', because it allows the layers below the surfaces to heat up. This temperature control was finished when the kinetic energy of the atoms near the interface did no longer change significantly, that means when the process of creating new bonds had finished. The specific factor was chosen such that the bulk layers could not cool down below the initial temperature. For a somewhat

smaller scaling factor the temperature of the bulk layers will be constant, yielding the same results as in the first approach. The energy which is removed by the rescaling procedures corresponds to a flow of kinetic energy into a macroscopic substrate. Within the first approach, the average kinetic energy at the borders of the simulated system remains constant whereas within the second approach the heat flow is chosen such that the temperature far away from the interface remains constant.
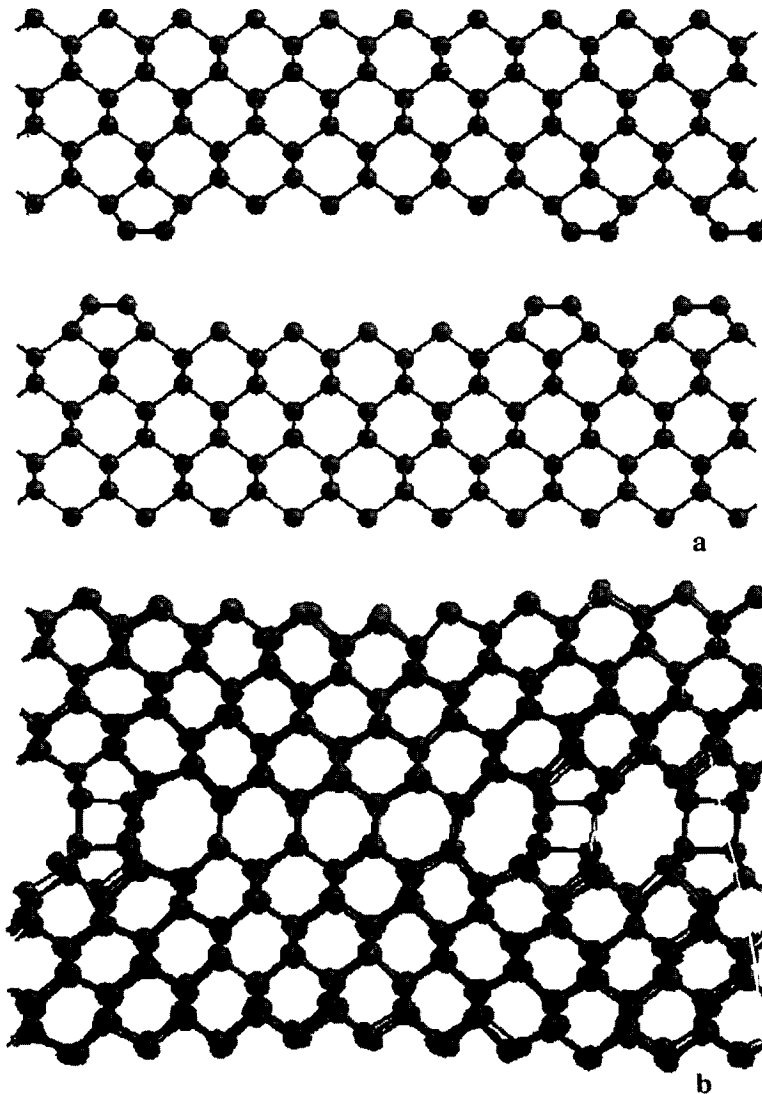
Fig. 4. MD-simulation of Si(100) wafer bonding of reconstructed surfaces with atomic-height steps. (a) Cross-section of the starting configuration, (b) snapshot at 10^{-12} s showing the contact of the lower terraces.

5. Perfect bonding

Fig. 3 shows the MD-simulations of wafer bonding for perfectly aligned smooth Si(100) faces, applying the slow heat approach. The starting configuration is shown in Fig. 3a, with the two opposite faces reconstructed in 2 × 1 patterns each. The distance of the dimer bonds is 3.8 Å so that initially there is a very weak attraction between the surfaces. Because of the attractive forces, the slabs move towards each other (Fig. 3b), with new 'bonds' forming. The energy released by the attraction of the surfaces causes the dimers to break up (Fig. 3c). The surface atoms find their bulk positions, before after some time the interface is almost perfectly bonded (Fig. 3d). Continuing the dynamics leads to the annealing of the imperfect regions still present.

6. Surface steps

To model a situation more closely related to experiments, the effect of surface steps is investigated in Fig. 4. Both opposite surfaces have a step of one atomic height, with the dimer bonds of the upper terrace perpendicular to the step (Fig. 4a). The upper and lower terraces are facing each other. Depending on the heat conduction approach, the behavior of the upper terraces is similar to the perfect bonding situation, whereas the behavior of the lower terraces corresponds to the so-called avalanche effect and is supposed to occur for any substrate thickness. The bonding of the lower terraces starts after the bonding of the upper ones, inducing an elastic deformation at the step and hence forcing the lower terrace atoms of one surface to approach to those on the other. At a
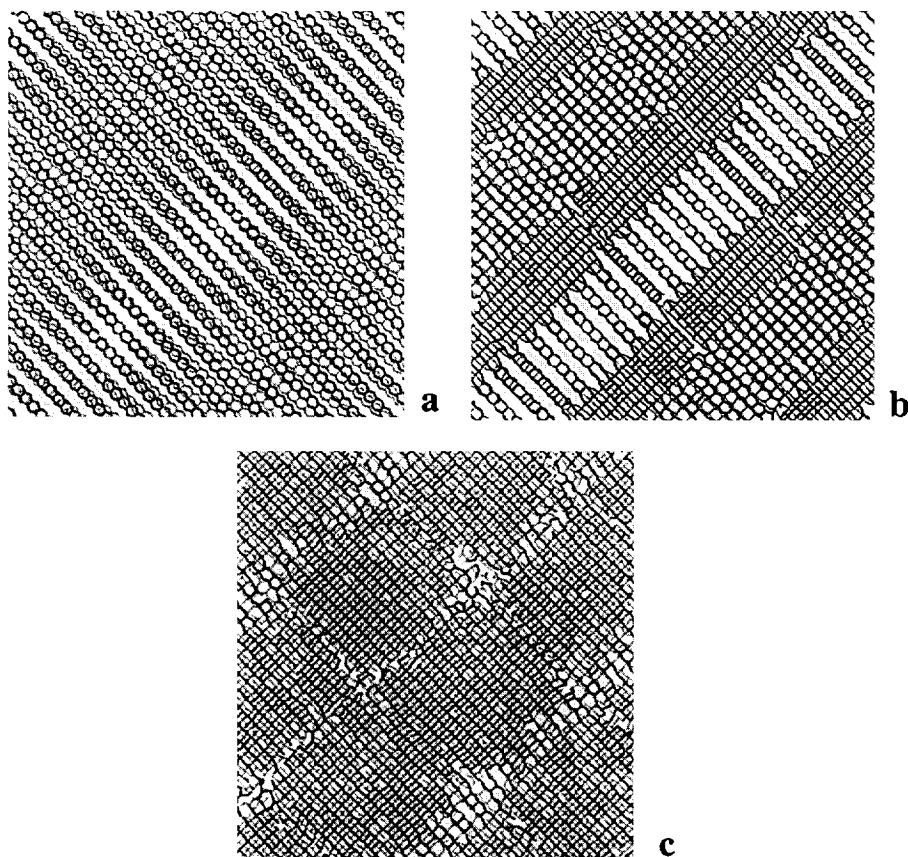

Fig. 5. MD-simulation of rotationally misoriented Si(100) wafer bonding, plane view with light (dark) lines for bonds of upper (lower) surface. (a) Starting configuration with 4.58° misorientation, (b) after 1.25 ps at 300 K, (c) after additionally 1.25 ps at 900 K and cooling down to RT.

certain point also the atoms on the lower terraces may interact and form a bonded interface (Fig. 4b). The energy gain owing to the creation of new covalent bonds is much higher than the energy necessary for a small elastic distortion of atoms from a tetrahedral configuration.

7. Misorientations

To study the effect of a small twist angle (Fig. 5), one surface is rotated by an angle of 4.58° corresponding to a $\Sigma = 313$ boundary. Fig. 5a shows a plane view of the starting configuration. Such a small twist angle may not occur in conventional growth processes, but the experimental wafer bonding equipment allows the combination of silicon wafers with any desired misorientation. With the surfaces closely approaching and bonds forming in between (with respect to an appropriate cut-off radius), three distinct regions occur at the interfaces (Fig. 5b): one in which the dimer rows of the upper surface lie in between those of the lower one, another one in which the dimer rows of the surfaces lie on top of each other, and a third one in which interface atoms have a bulk-like environment. Probably, the crystalline regions will grow slowly during a long time-run. In order to accelerate the growth of

the crystalline regions, the simulation was continued at 900 K before the system was cooled down again (Fig. 5c). Now, almost all atoms have a bulk-like environment, these regions are separated by dislocations. Fig. 6 shows the simulated 400 kV HREM images of the bonded interface with rotational misorientations for different defoci. In 110-direction a fringe contrast occurs very similar to the experimental observations: columns of atom pairs periodically disturbed by the diffraction contrast according to elastic strain. However, for all defocus values chosen no additional fringes are directly obtained. Image filtering shows additional fringes solely parallel to the interfaces, probably because the model is too small for correct image calculations.

8. Conclusions

Molecular dynamic simulations based on a modified Stillinger–Weber potential are used to investigate the elementary steps of bonding two Si(001) wafers. The potential has to be rescaled generating almost instantaneously a fully symmetrically dimerized surface. The energy dissipation and thus the dynamic bonding behavior are controlled by the transfer rates for the kinetic energy. The applicability of the method is demonstrated by studying the inter-
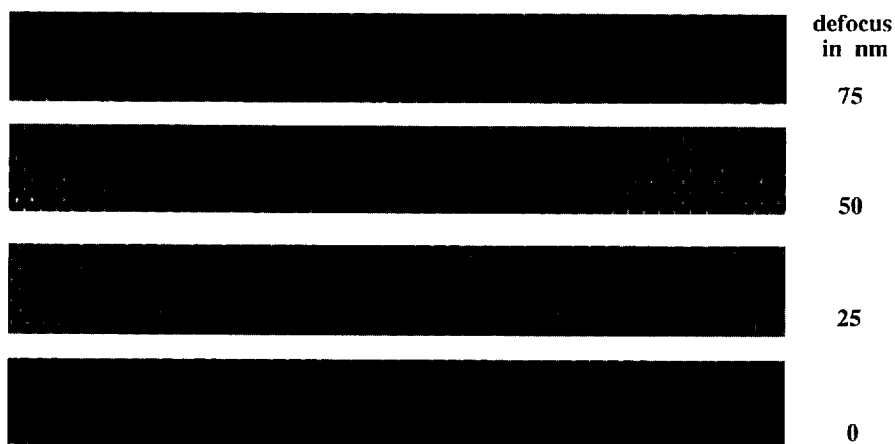

defocus in nm

75

50

25

0

Fig. 6. Simulated 400 kV (110)-HREM micrographs (defocus series), MD-calculation of bonded Si(100) wafers with misorientation (4.58°, imaging: $C_s = 1$ mm, $\delta = 8$ nm, $\alpha = 16^{-1}$ nm, $\alpha_D = 0.5$ mrad).

action of perfect wafer surfaces, which corresponds to UHV bonding conditions. First calculations covering the influence of surface steps, rotational misorientations and adsorbates are being carried out to correlate atomic properties with macroscopic ones. MD simulations showed that the most crucial problem consists in finding complex atomic potentials covering bulk and surface structures as well as the interaction with adsorbates and the correct hydrophobic or hydrophilic termination. HREM imaging is a suitable tool to investigate interfaces at an atomic level.

References

[1] K. Scheerschmidt, S. Ruvimov, P. Werner, A. Höpner and J. Heydenreich, J. Microsc. 179 (1995) 214–228.
[2] S. Ruvimov and K. Scheerschmidt, Phys. Status Solidi (a) 150 (1995) 471–478.
[3] D. Timpel and K. Scheerschmidt, Phys. Status Solidi (a) 150 (1995) 51–63.
[4] U. Gösele, H. Stenzel, T. Martini, J. Steinkirchner, D. Conrad and K. Scheerschmidt, Appl. Phys. Lett. 67(24) (1995) 3614–3616.
[5] D. Conrad, K. Scheerschmidt and U. Gösele, Appl. Phys. A 62 (1996) 7–12.