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Computational Materials Science 9 (1997) 108–115

COMPUTATIONAL MATERIALS SCIENCE

Molecular dynamics modelling of silicon wafer bonding

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Abstract

Molecular dynamics simulations based on empirical potentials are used to investigate the elementary steps of bonding two Si(001) wafers. The resulting interface models are applied to analyse high resolution electron microscopy structure images of perfectly bonded wafers (UHV conditions). © 1997 Elsevier Science B.V.

PACS: 02.70.Ns; 34.20; 68.35

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

1. Introduction

Molecular dynamics provides a tool suitable for simulating time-depending processes at an atomic level as, for example, the growth of crystals, the reordering of interfaces, the interaction between adatoms and surfaces, as well as the relaxation of core structures of lattice defects. Classical molecular dynamics (MD) solves the equations of motion of an ensemble of particles assuming suitable interatomic potentials and boundary conditions. The simulation of macroscopically relevant structures here requires a large number of particles to be considered and many-body empirical potentials to be applied.

Silicon wafer bonding has increasingly become a promising technology for silicon-on-insulator and micromechanical applications. Starting with adhesively bonded materials the covalent interaction of two wafers usually needs some thermal treatment. UHV-experiments, however, demonstrate the possibility of large-area covalent Si wafer bonding at room temperature [1]. Bonding energy and forces strongly depend on the surface structure (native oxides, adsorbates, hydrophobic or hydrophilic termination) and the bonding control equipment (atmospheric or ultrahigh vacuum bonding, annealing temperature and time). To better understand the physical processes of wafer bonding the experimental investigations are supported by theoretical analyses of the interaction of the atoms at the two surfaces contacting each other by using MD structure modelling [2]. High voltage and high resolution electron microscopy (HREM) structure imaging was applied to investigate the resulting interfaces and the defect structures at an atomic level (see, for example, Refs. [3–5]).

2. Molecular dynamics simulations of wafer bonding

The interatomic forces in covalent solids can completely be described only if the influence of the local environment according to the quantum electronic structure is also included. However, empirical

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PII S0927-0256(97)00064-5

potentials have been developed, which allows one to simulate the non-local many-body interaction sufficiently well, thus enabling the application of long-time MD simulations to larger systems as it is necessary to investigate, for example, the wafer bonding interaction processes. In agreement with ab initio pseudopotential calculations, the potential of Tersoff predicts the asymmetric reconstruction with fourfold coordinated atoms at interfaces with defects. Therefore the potential of Tersoff was applied to investigate the core of 60° partial dislocations in Si and other defects left after the bonding of two wafers [6]. Because of the short range of the Tersoff potential it was supposed here that the bond topology is already prescribed by the usual process starting with separated Si blocks of suitable surface structure and orientation (surface reconstruction, steps and adsorbates) and applying long-range potentials. The potential most often used for group IV semiconductors is the Stillinger–Weber potential, with a smooth cut-off behind the nearest neighbour distance, and which is scaled with respect to the cohesive energy, the lattice constant and the melting point. In contrast to the Tersoff potential it supports a symmetric quasi-fivefold coordinated reconstruction at interfaces [6]. The Stillinger–Weber potential, however, allows the second next neighbour interaction to be included, which is a presupposition to the simulation of the dynamical behaviour without preordered surfaces and prescribed topology. The interaction of two silicon surfaces can be studied solely by correctly revealing the 2×1 reconstruction of a clean Si(100) surface. Thus, as a first improvement, the potential has to be rescaled to the second next neighbour interaction generating almost instantaneously a fully symmetrically dimerized surface within a few 100 fs and showing energy gain and bond length in good agreement with ab initio results [2].

The second improvement is related to the energy transfer, because each new bond implies an energy gain of the order of eV, which in a constant energy simulation is distributed to a small number of atoms resulting in an inappropriate melt of the surfaces. The energy dissipation and thus the dynamic bonding behaviour are controlled by the transfer rates of the kinetic energy at the borders of the model describing an energy flux into a macroscopic substrate. Two approaches are applied to rescale every 100 time steps the averaged velocities of the outermost atomic layers either down to a constant temperature (fast heat transfer), or by using a constant reduction factor (slow heat transfer). A more frequent rescaling would affect the lattice vibrations. Within the fast heat transfer approach, the average kinetic energy at the borders of the simulated system remains constant whereas within the slow heat conduction the flux is controlled such that the temperature far away from the interface remains constant.

3. Results of MD simulations

The molecular dynamics simulation starting with two perfect and parallel-oriented Si blocks with perfectly aligned 2×1 reconstructed (100) surfaces and applying the slow heat transfer approach yields perfectly bonded structures, i.e. it recovers an ideal crystal [2]. However, a fast heat transfer, a starting configuration, with the dimer rows in orthogonal domain orientation, or including steps or small rotational misorientations, result in configurations no longer perfectly coordinated. As shown in [2], the effect of a small twist angle as a rotational misorientation without other defects at the surface, results in a mosaic-like interface structure. After sufficient relaxation under slow heat transfer conditions almost all atoms have a bulk-like environment separated by misfit dislocations, which may have a high rate of kinks. Similar structures are obtained for adsorbates, or by simulating the bond process of different materials, which will be reported elsewhere. The present investigations are restricted to clean (100) Si surfaces with 2×1 dimer domain structures in parallel or orthogonal orientation, without or with surface steps.

Fig. 1 shows two metastable configurations (Fig. 1a–d) and an equilibrium one (Fig. 1e and f) in different viewing directions: the $[1\bar{1}0]$ projection (Fig. 1a, c and e) and the [110] projection (Fig. 1b, d and f). The first example (Fig. 1a and b) displays the resulting bonded structure of perfectly oriented crystals within a fast heat conduction approach, i.e. the energy is removed by rescaling the velocities of the five outermost atomic layers of each slab to the fixed temperature of 300 K. To obtain the equilibrium atomic positions the structure is slowly cooled down

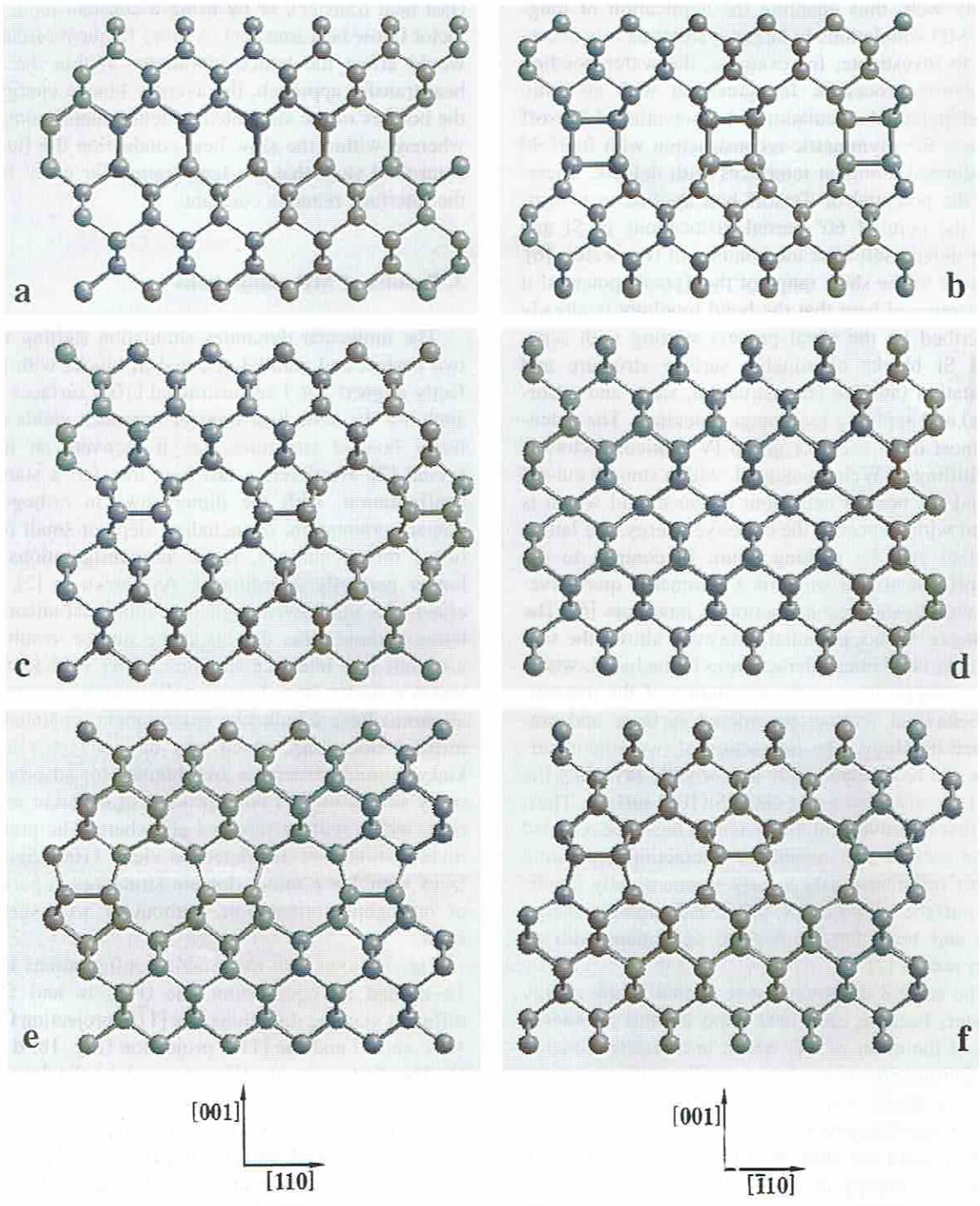

Fig. 1. MD relaxed interface structures of bonded Si(001) interfaces, [$\bar{1}$10] and [110] projections: (a, b) parallel dimers, fast heat, Stillinger–Weber, (c, d) orthogonal dimers, slow heat, Stillinger–Weber, (e, f) dito with Tersoff.

to 0 K after more than 1 ps MD run with no further changes of the structure. The energy of the interface is 1.54 J m^{-2}, the structure is not perfect because the dimers are still bonded, nevertheless the atoms are fourfold coordinated. Starting with a 90° rotation of the original surfaces (Fig. 1b and d), i.e. with an orthogonal dimer orientation of the 2×1 reconstructed (001) surface, which corresponds to a 90° twist boundary and using the Stillinger–Weber potential, the dimers of only one surface are broken during the MD run. A metastable fivefold coordinated interface is created, i.e. showing coordination defects, with an energy of 1.04 or 1.02 J m^{-2} in terms of the Stillinger–Weber or Tersoff potential, respectively. The structure is symmetrical with respect to the interface and can be characterized by a Pmm(m) layer group symmetry. The relaxation of the same configuration through the Tersoff potential is shown in Fig. 1e and f. Here, the grain boundary region is (2×2) reconstructed and can be imagined to consist of arrays of structural units, with fourteen atoms forming eight five-membered rings. It has the improper symmetry axis $\bar{4}$ and belongs to the point group $\bar{4}2m$ (D_{2d}), called the $\bar{4}2m$-dreidl [6], which is a new structural unit with edges in terms of bonds. The dreidl fits two rotated half crystals of minimal structural disorder and fourfold coordination described by P($\bar{4}$)m2 layer symmetry. The interface energy is 0.81 J m^{-2} (0.85 J m^{-2} for Tersoff energy calculation), only the dimer bonds of 0.244 nm in length are moderately stretched.

Studying the energy flux at surfaces with atomic steps (see Fig. 2) allows one to investigate the restrictions on the bonding process of more realistic surfaces, which are stepped. In Fig. 2 the grey level describes the potential energy above the ground state, which is dark. The upper terraces behave like perfect surfaces (Fig. 2a): Starting with dimerized surfaces, a weak attraction owing to the next neighbour interaction initiates the dimers to rearrange and to create new bonds. The energy the bonds have gained dissipates (Fig. 2b) increasing the kinetic and elastic

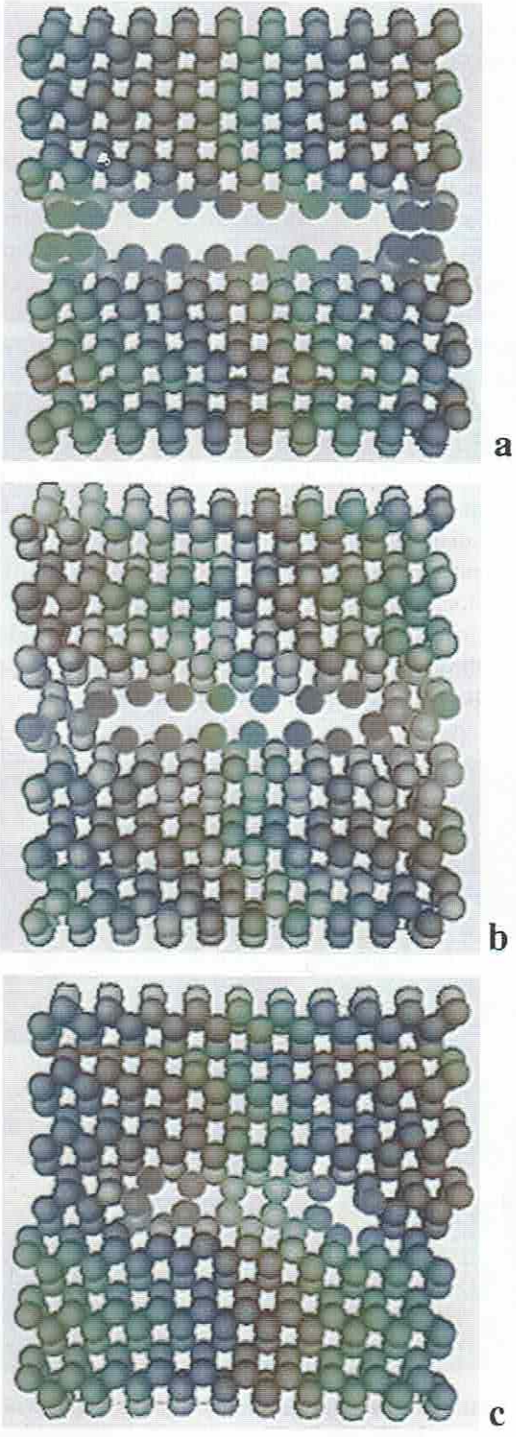

Fig. 2. Energy dissipation during bonding at steps (slow heat transfer, light grey indicating higher potential energy above ground state): (a) initial configuration, (b) after 12.5 fs (300 K), (c) after cooling (0 K).

energies of the bulk. If the heat transfer is slow enough, the resulting avalanche effect implies the bonding of the lower terraces, too. However, after relaxation through the Stillinger–Weber potential a disturbed interface and defects are left similar to dissociated partial dislocations (cf. Fig. 2c). Fig. 3 shows resulting interface structures of wafer bonding with steps for which the relaxation is continued through the Tersoff potential. Single layer steps rotate the dimerization direction in the neighbouring domains and give rise to a stacking fault of either intrinsic (Fig. 3a) or extrinsic (Fig. 3b) type, depending on the dimer orientation in the adjacent terraces. Thus the interfaces between, or outside, the single-layer steps are characterized by the 90° twist-rotation discussed in Fig. 1e and f, which corresponds with the starting configuration due to step types S_A or S_B, respectively. The double-layer step does not change the dimer orientation and may finally relax to 60° partial dislocations. Depending on the possibility of rigid body translations between the steps, the shuffle-set dislocations can be accompanied by a row of vacancies as shown in Fig. 3c. The slow heat relaxation through the Tersoff potential results in perfectly bonded interfaces between the steps.

4. Ultrahigh vacuum wafer bonding

Mirror-polished and smooth pieces of solids adhere to each other provided there are no dust particles between their surfaces. This is well known and holds good of a large number of materials. Both hydrophilic and hydrophobic wafer bonding at room temperatures, however, imply rather weak bonding energies (van der Waals forces). Covalent bonding yielding high bonding energies is attained by annealing the room-temperature bonded wafers at high temperatures ($\geq$ 1000°C). For a number of applications and especially to investigate the physical processes of wafer bonding itself it is important that the bulk bond strength can be reached by room temperature bonding without any additional heating step. Ultrahigh vacuum (UHV) experiments demonstrate that large-area, self-propagating, room-temperature covalent wafer bonding of commercially available (100) silicon wafers is possible [1]. After removal of the native oxide by hydrofluoric acid, rendering the surfaces hydrophobic and covered with hydrogen, the wafers were bonded as usual in a microclean room. In the UHV-chamber, the bonded wafers were separated and the hydrogen was removed by heating

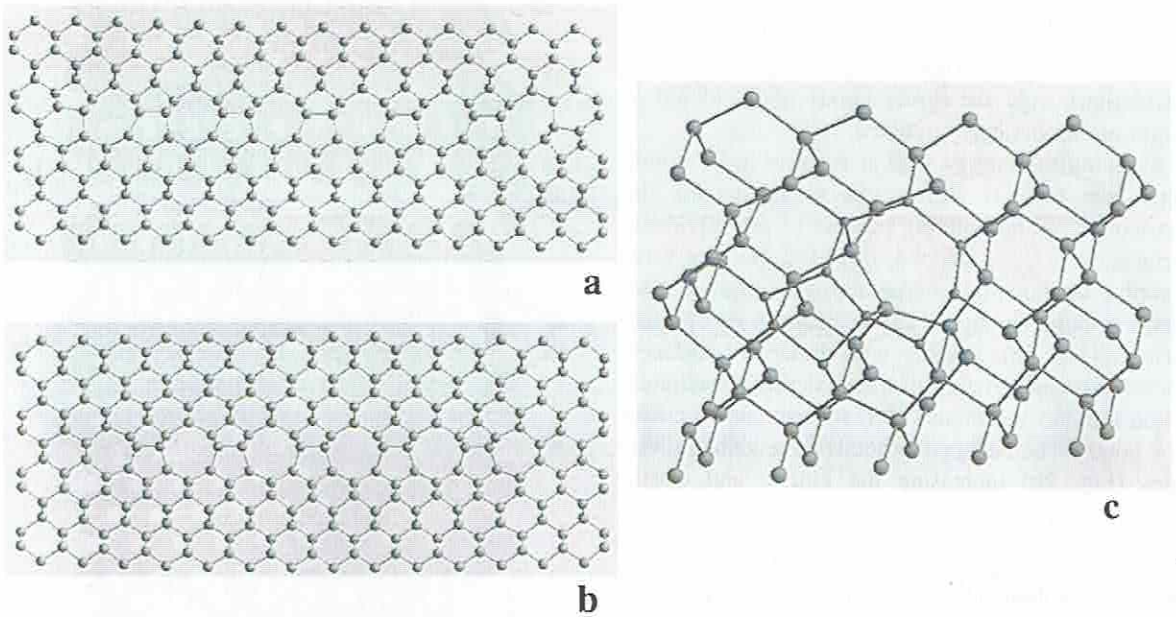

Fig. 3. MD relaxed structures after bonding at steps: (a) intrinsic, (b) extrinsic stacking fault (single layer steps), (c) 60° dislocation and line of vacancies (double steps).

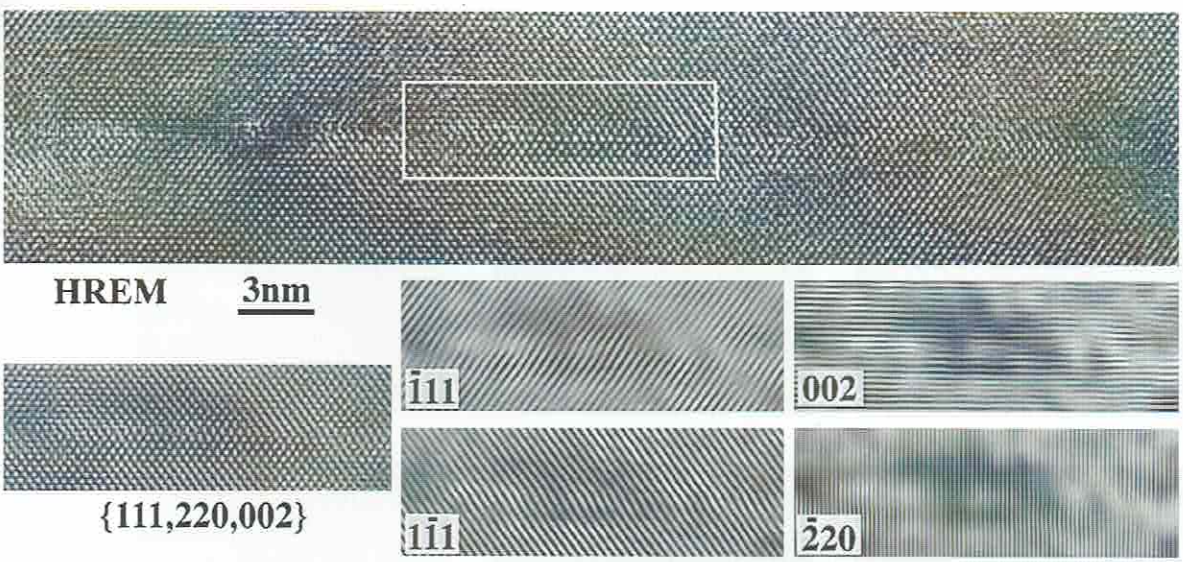

Fig. 4. UHV bonded Si(001) wafers: 200 kV [110]-HREM and filtered images.

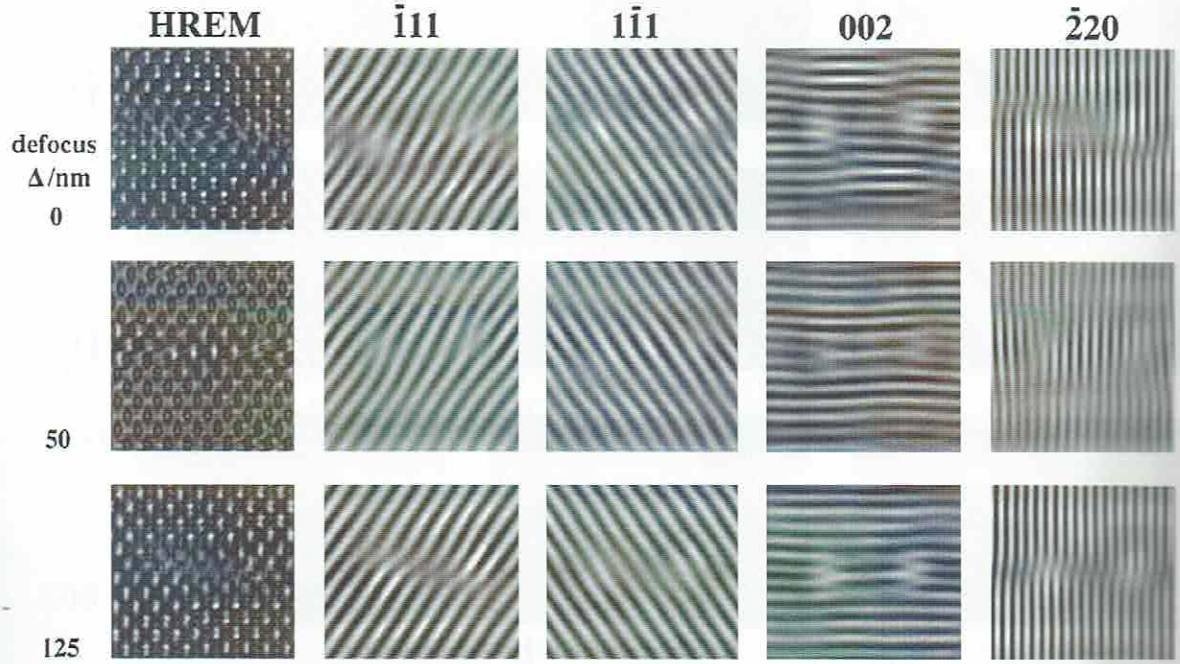

Fig. 5. MD simulated (001)-Si wafer bonding at double steps: theoretical 200 kV-[110]-HREM and filtered images (spherical aberration = 1 mm, defocus spread = 1 nm, beam divergence = 0.05 mrad, thickness = 7.9 nm).

and pumping. After cooling to room temperature within the UHV-chamber the bonding was initiated by an appropriate manipulator in the centre of the wafer.

Fig. 4 shows the resulting structure, viz. the example of an interface of room-temperature UHV-bonded silicon wafers investigated by cross-sectional HREM (Fig. 4a, 200 kV, [110] orientation). Though

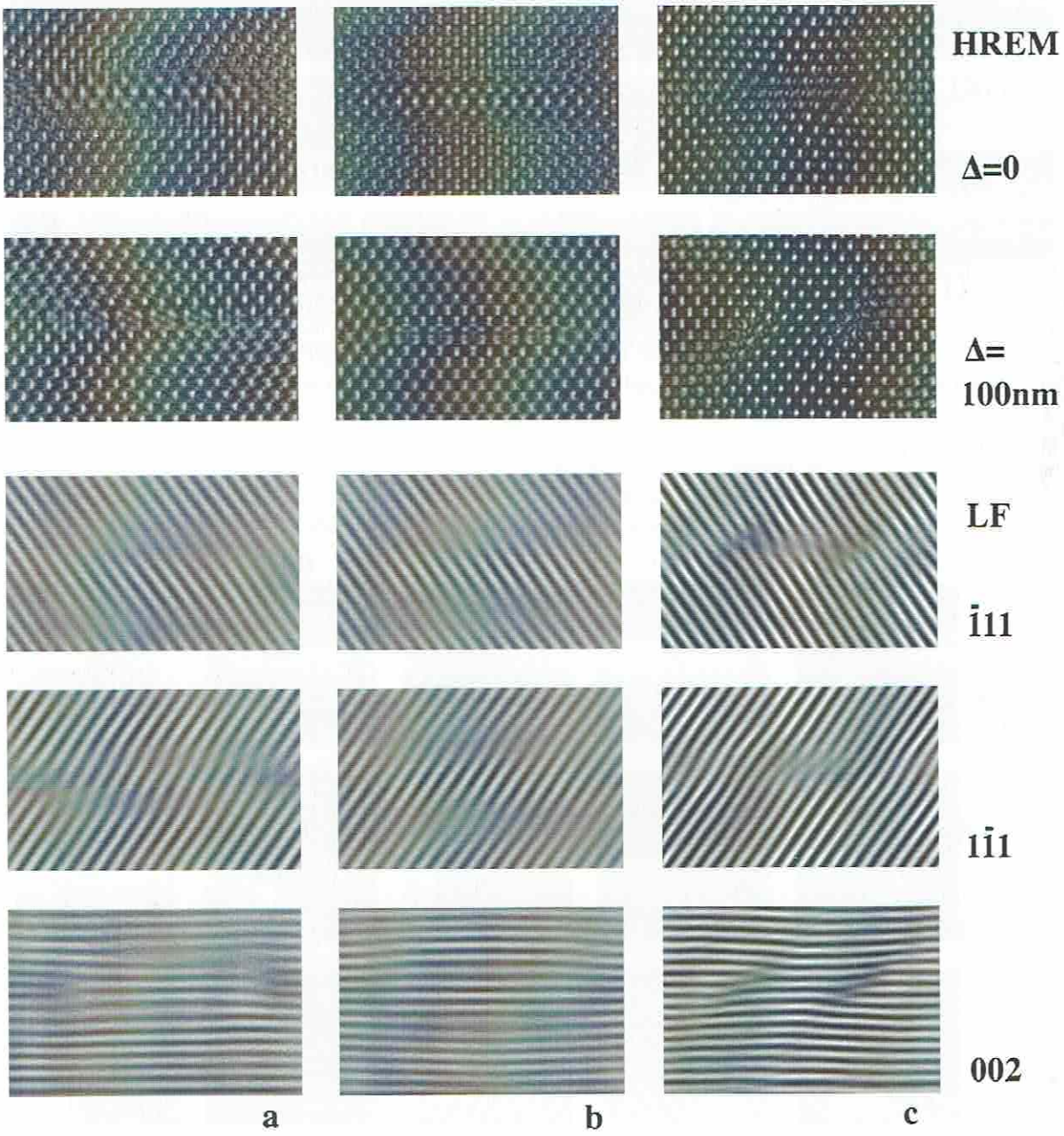

Fig. 6. Simulated 200 kV-[110]-HREM and filtered images: (a) intrinsic, (b) extrinsic stacking faults (single steps), (c) dislocation with line of vacancies (double step, thickness = 6.1 nm, defocus Δ).

not showing any noticeable intermediate layer the interface does not correspond to a perfect structure. Along the interface darker diffraction contrast regions occur at distances of about 5–7 nm. This may be due to incomplete bonding processes arising from misorientations of the two wafers, fast energy dissipation, or defects left behind at surface structures as, for example, at surface steps. The corresponding images filtered of the selection marked (Fig. 4b to f, for a 'low pass filter' and the 'lattice fringe images' of reflection pairs $\bar{1}11$, $1\bar{1}1$, 002 and $2\bar{2}0$, respectively) show additional lattice planes indicating interfacial dislocations. For comparison, simulated HREM images of bonded interfaces with steps are given in Figs. 5 and 6. Fig. 5 shows a simulated defocus series of the metastable double-layer step according to Fig. 2c. Both the HREM images and the filtered 'lattice fringe' images demonstrate the strong influence of the imaging conditions on the contrast details obtained. HREM images of the (100) intrinsic and extrinsic stacking faults according to Fig. 3a and b simulated for the Gauss-focus ($\Delta = 0$) and the under focus $\Delta = 100$ nm, are illustrated in Fig. 6a and b. These images and the corresponding filtered 'lattice fringe' micrographs demonstrate that the effect of the (2×2) reconstruction on the image contrast (a double contrast periodicity with respect to the perfect lattice contrast) can be enhanced or suppressed by choosing the appropriate defocus values.

5. Conclusions

Molecular dynamics simulations based on a modified Stillinger–Weber potential were used to investigate the elementary steps of bonding two Si(001) wafers. Bonded structures including surface steps were additionally refined by simulating the relaxation through empirical Tersoff potentials. The applicability of the method has been demonstrated by studying the interaction of wafer surfaces without adsorbates, which corresponds to UHV bonding conditions. Calculations covering the influence of surface steps, rotational misorientations and adsorbates were 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, etc. For the perfectly aligned, adsorbate free surfaces, the most stable configurations can be proposed using a new type of structural unit. Depending on the type of reconstruction and the energy transfer, expansion or contraction of bonds as well as metastable configurations are obtained. For non-restricted relaxation, the boundaries tend to optimize the angular bond distortions because the most important factor is the directionality of the bonds.

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