Atomic Structure of Twist Bonded Interfaces: A Molecular Dynamics Study

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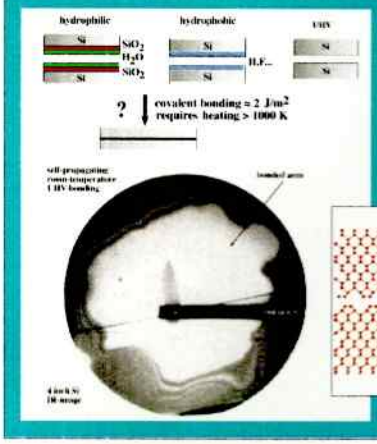
MOTIVATION: WAFER BONDING PROCESSES

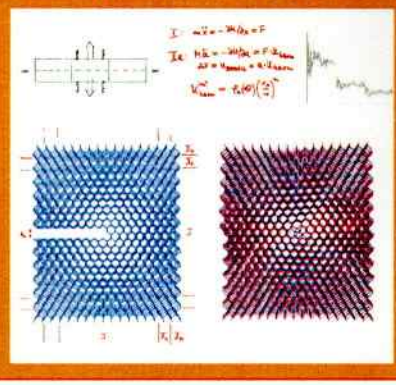


- atomic level processes
- defects and adsorbates
- misalignment
- miscut and steps
- interface structure
- bondability
- mechanics / electrics

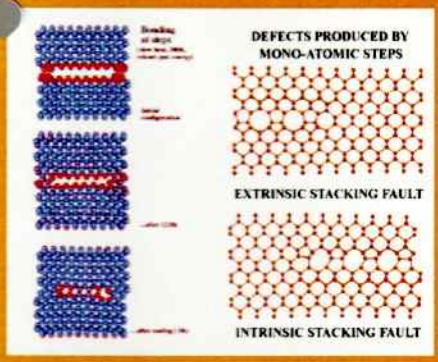
METHOD: CLASSICAL MOLECULAR DYNAMICS

Integrating 3N-Newtonian Equations for N>10000 particles using time steps of some fs

- geometric start model
- initial Boltzmann momenta
- NVE, NpT, Nose-bath,...
- free, fixed, periodic, or elastic boundary conditions
- Tersoff, MEAM or analytic Bond Order Potentials (second moment tight binding) fitted to macroscopic and ab initio properties

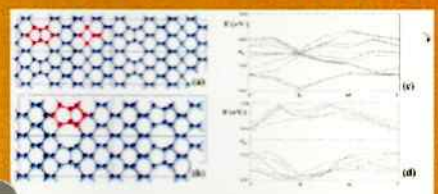


BONDING ACROSS SURFACE STEPS



- bonding over monatomic steps yields 90 degree twist boundaries
- bonding at double steps needs slow heat conduction and results in 60-degree dislocations with eventually attached rows of vacancies separated by a perfect interface

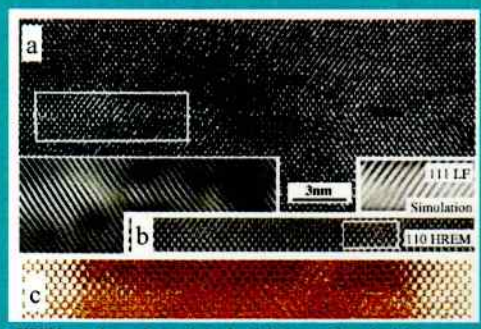
ELECTRONIC INTERFACE STRUCTURE OF 90 DEGREE TWIST



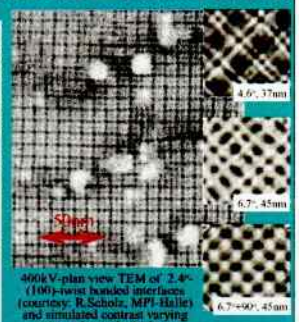
[110] projections (a,b) and bandstructures (c,d) of bonded 90 dgr twist boundaries: (a,c) Pmmm(m), (b,d) P(4)m2 dreidl

- both the metastable semimetal interface and the dreidl structure are confirmed by DFT calculations
- possibility of band gap tailoring ?

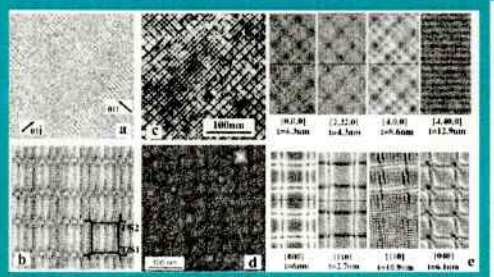
BONDING WITH SMALL TWIST ROTATIONS: SCREW DISLOCATIONS



HREM experimental (a) and simulated (b) images from the 4.6 degree twist bonded model (c) and filtered selections showing fringe termination

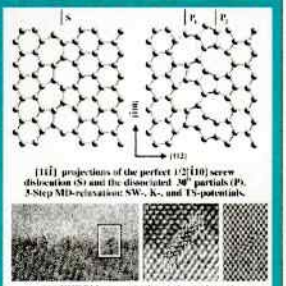


400kV-plan view TEM of 2.4° (100)-twist bonded interfaces (courtesy: R.Scholz, MPI-Halle) and simulated contrast varying twist and sample thickness



100-projections of twist bonded MD-models (a: 4.6 degree, b: perfect screws) and plan view TEM experiments (c,d), simulated thickness and tilt series (e)

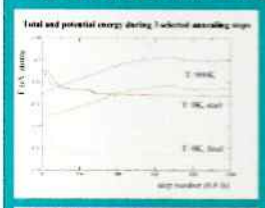
SCREW DISSOCIATION

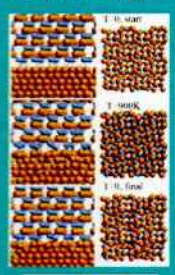


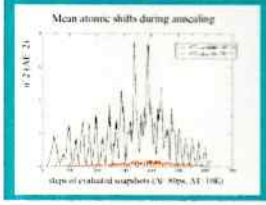
[1$\bar{1}$1] projections of the perfect 1/2[$\bar{1}$10] screw dislocation (S) and the dissociated 30° partials (P). 5-Step MD-relaxation: SW-, K-, and TS-potentials.

110-XHREM of a wafer bonded twist boundary: Intrinsic stacking fault ribbon bounded by two 30° partials. Simulation: MD-relaxed,200kV,Cs=1mm,Scherzer,t=1.56nm.

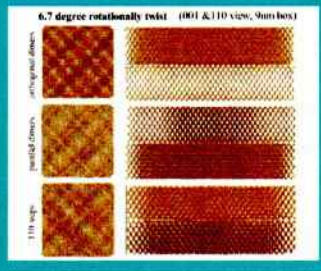
EXAMPLE: 12.8 DEGREE TWIST BONDING OF SI/SIGE WITH FREE BOUNDARIES



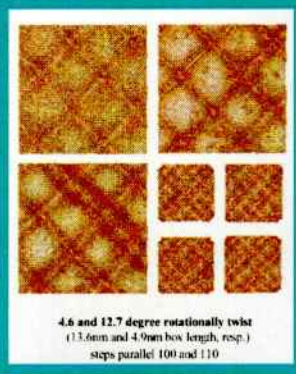




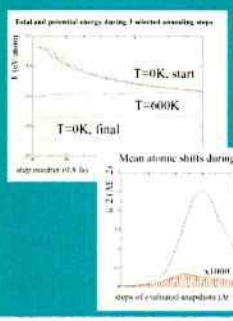
VARIATION OF TWIST ANGLE: VARYING DEFECT STRUCTURE

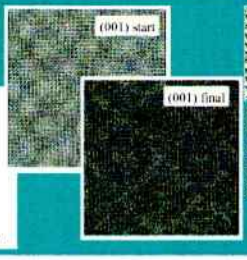


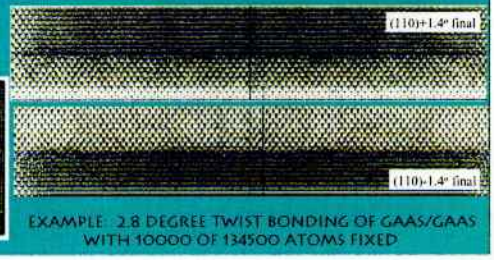
α(degree)	ΔE(eV/atom)	atoms	box(nm)
2.8 Σ841	0.4	134500	22.3
4.6 Σ313	0.5	40000	13.5
6.7 Σ145	0.3	23000	9.2
12.7 Σ41	0.2	6500	4.1



4.6 and 12.7 degree rotationally twist (13.6nm and 4.9nm box length, resp.) steps parallel 100 and 110







EXAMPLE: 2.8 DEGREE TWIST BONDING OF GAAS/GAAS WITH 10000 OF 134500 ATOMS FIXED

ATOMIC STRUCTURE OF TWIST BONDED INTERFACES: A MOLECULAR DYNAMICS STUDY

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Abstract

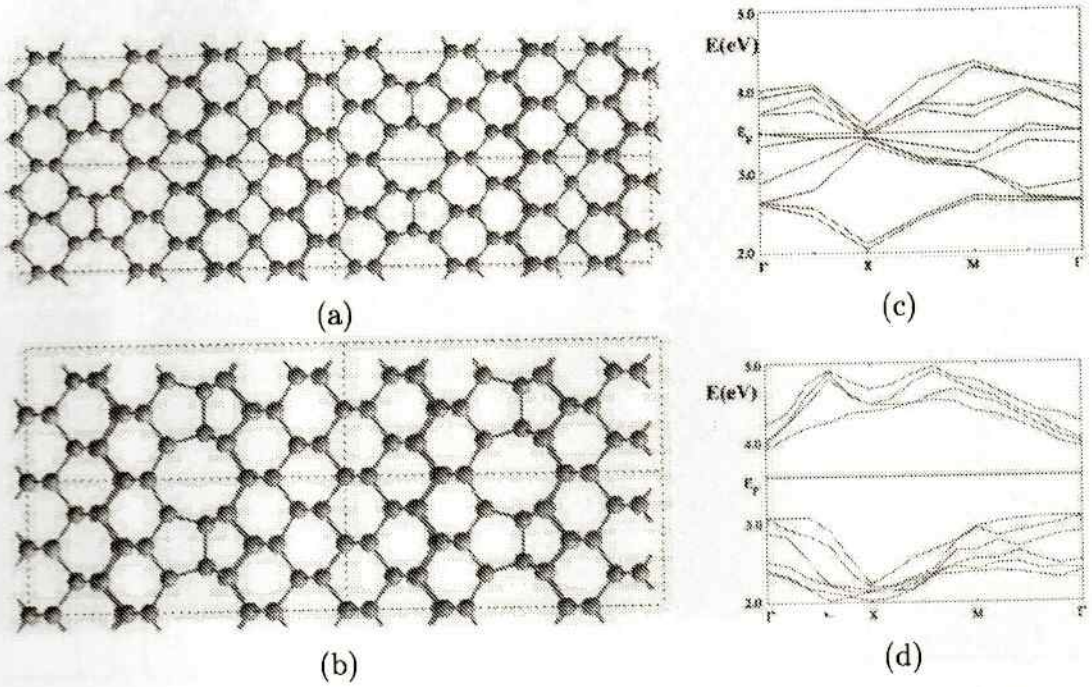
Molecular dynamics simulations using empirical potentials have been performed to describe atomic interactions at interfaces created by macroscopic wafer bonding. Misalignment due to relative twist rotation of the wafers influences the bondability of larger areas. Depending on the twist angle the bond energy varies 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.

Introduction

Wafer bonding, i.e. the creation of interfaces by joining two wafer surfaces, has become an attractive method for many practical applications in microelectronics, micromechanics or optoelectronics. The macroscopic properties of bonded materials are mainly determined 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 support the experimental investigations or to predict the bonding behavior.

It is possible to use quantum-theoretical ab initio calculations with a minimum of free parameters to predict material properties of small systems. The only practical method to simulate atomic processes with macroscopic relevance, however, is classical molecular dynamics (MD) using suitably fitted empirical many-body potentials. Basically, MD integrates the Newtonian equation of motion with a fifth-order predictor-corrector algorithm using time steps in the order of fs. The procedure used here is outlined e.g in [1] together with further references of succesfully applying MD-simulations to wafer bonding. Such simulations make a sufficiently large number

of particles and relaxation times up to μs accessible, though the electronic structure and the nature of the covalent bonds can only be described indirectly. However, it is important to find physically motivated semi-empirical potentials, starting mostly with the moments of the electron density and using tight-binding representations (cf. e.g. [2]).



(a) (c)

(b) (d)

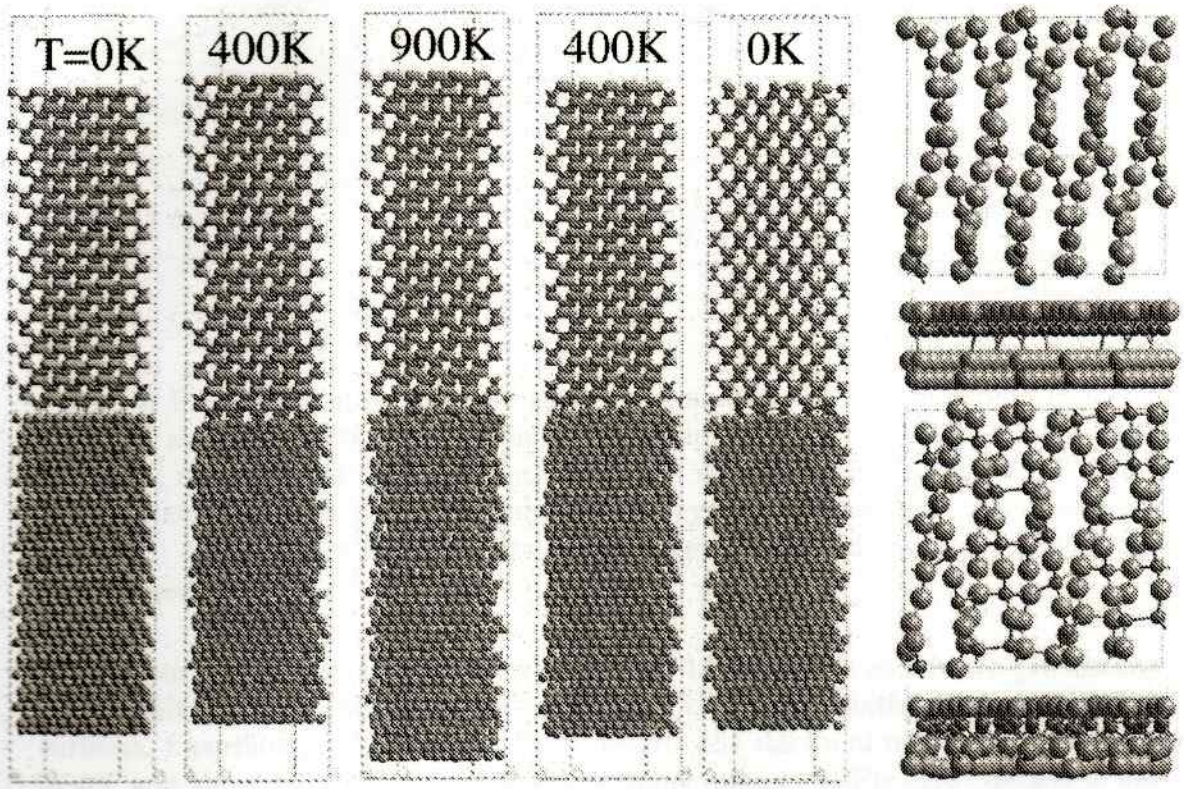
Figure 1: MD simulated structural model (a) of the $Pmm(m)$ interface at 90° twist, (b) of the $P(\overline{4})m2$ interface at 90° twist, and corresponding DFT band structures (c,d), respectively

Whereas bonding of two perfectly aligned, identical 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 are created. Bonding wafers with rotational twist leads additionally to a network of screw dislocations at the interface. The present paper investigates the interface bonding of silicon wafers as a function of the twist angle and the thickness of the wafers in more detail. In addition the transferability of the results to the systems Si/SiGe and GaAs/GaAs with very similar bonding behavior is also demonstrated.

The bonded interface with 90° twist rotation

Misalignment of the wafers during bonding yields bonded interfaces with twist rotation. A special situation is the 90° twist, which always occurs between monoatomic steps. A Stillinger-Weber potential applied to a 90° twist bonded wafer pair [1] yields a metastable fivefold coordinated interface with a mirror symmetry normal to the interface characterized by a Pmm(m) layer group (cf. Fig. 1(a)). Using the Tersoff or BOP-like potentials (cf. e.g. [2]) and metastable or well-prepared starting configurations allows further structure relaxation and energy minimization. Figure 1(b) shows

this relaxed configuration, which is (2x2) reconstructed and consists of structural units with a $\bar{4}2m$-(D2d) point group symmetry, called the $\bar{4}2m$-dreidl.



(a) (b)

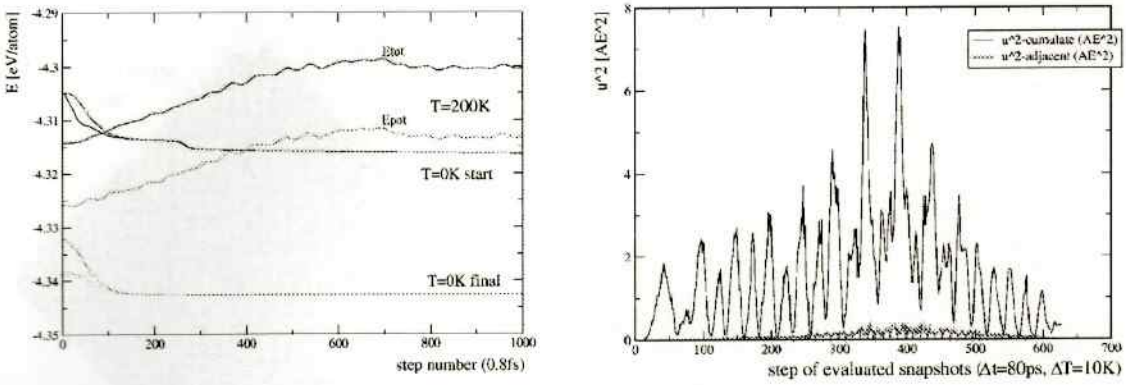
Figure 2: Snapshots (a) and interface details (b; top: start, bottom: final configuration at 0K, [001] and [110] views, resp.) selected from MD simulations of bonding and annealing Si with SiGe wafers with a large rotationally twist angle of 22.6° to demonstrate the oscillatory avalanche effect: 2080 atoms, 2x2x13 nm box, free boundaries.

It should be emphasized that the dreidl structure is found to be the minimum energy configuration also in DFT-LDA simulations [1]. However, the energies differ from those given in [3]. Much more important is the modification of the band structure due to the different interface relaxation which may enable tailoring of the electronic properties. Whereas the metastable configuration (cf. Fig. 1(c)) yields semi-metallic behavior, the dreidl structure (cf. Fig. 1(d)) yields a larger band

Wafer bonding with small twist misalignment

The effect of a small twist angle as a rotational misorientation results in a checkerboard-like interface structure [5]. The simulation of wafer bonding starts with two perfect Si blocks (or the respective material considered) that are separated by a few Å and may have dimerized (100)-surfaces. gap than in perfect lattices.

For the sake of simplicity Fig. 2 demonstrates the wafer bonding of a Si/SiGe interface with a large twist angle of 22.6°, which needs only a very small simulation box to guarantee the periodic continuation along the interface region (2080 atoms,



(a) (b)

Figure 3: Energy and atom shifts for the MD simulation of the model from Fig. 2: (a) Potential and total energy as function of the simulation time for three selected annealing steps, relaxation at 0K for the start and the relaxed configuration and at 900K, the difference between potential and total energy characterizes the system temperature, (b) Mean square atomic shifts of subsequent evaluated snapshots, cumulated versus absolute shifts.

2x2x13 nm box). The boxlength is chosen here 13 nm which enables to get already good results without any additional restrictions, i.e. the simulation is made with free surfaces. Snapshots of the bonding are shown for the start and relaxed configuration at 0K and three selected intermediate annealing states. In Fig. 2(b) details of the interface are shown presenting only the adjacent layers of the start and the relaxed configuration in [001] and in nearly [110] view. Two effects are clearly demonstrated here. Because of using the lattice constant of Si for both wafer parts in the start configuration of the MD annealing cycle, the whole structure shows large oscillations and an avalanche effect to find out the equilibrium configuration, which is not restricted due to the free surfaces assumed. The rearrangements of bonds happens immediately in the first two layers near the interface by equally distributing the displacements and reordering such that the perfect coordination as within the bulk is preferred.

Fig. 3 shows the behavior of the potential and the total energy (a) and of the mean atomic displacements (b) for the annealing of the interface of Fig. 2. The final configuration has the lowered potential energy, i.e. by gaining approximately 0.028eV per atom the relaxed configuration is the more stable one. The difference between the total and the potential energy characterizes the temperature of the system reached, shown here for the step T=200K heating up. The structural oscillations are clearly reflected in the mean atomic shifts, too. Whereas the mean atomic shifts from step to step only reflect the moveability per integration step, the accumulated shifts describe diffusion, relaxation, and the thermic vibration according to the Debye-Waller factor.

Fig. 4 shows some of the resulting minimum structures for (001)-Si/Si wafer bonded interfaces 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

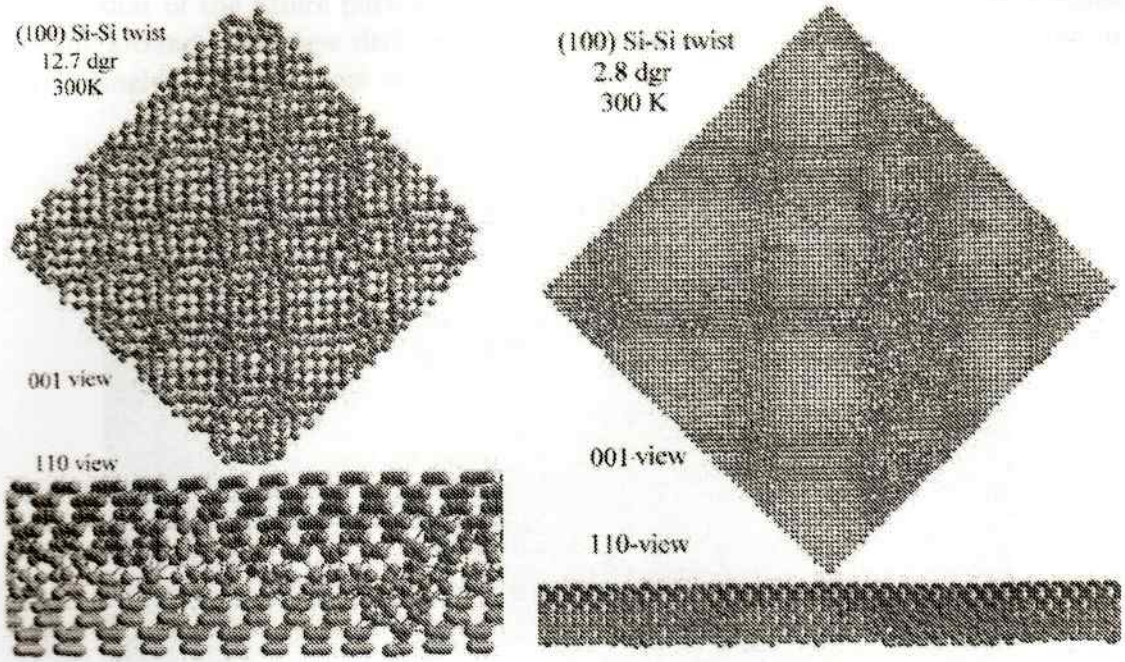


Figure 4: MD simulated structural models ([001] and [110] views) of bonded wafers with different rotationally twist angles annealed at 300K for parallel dimer start configurations: (a) 12.7°, 6500 atoms, 4.9nm box; (b) 2.8°, 134500 atoms, 22nm box, and with additional bonding over steps.

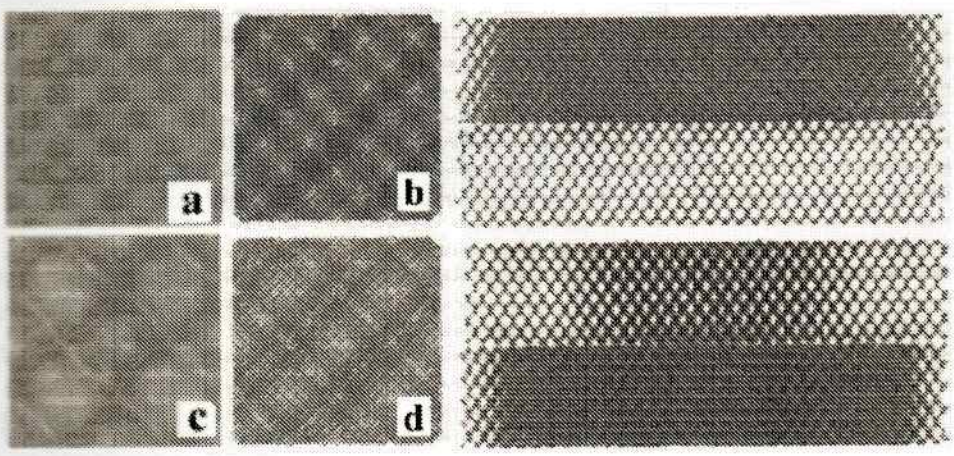


Figure 5: MD relaxations of bonding rotationally twisted wafers ([001] and [110] views) with different angles: a) 2.8°, 22nm box, orthogonal dimers, b) 6.7°, 9.2nm box, orthogonal dimers, [001] and [110] views; c) as a) and d) as b) with parallel dimers.

a high rate of kinks. The screw dislocation network of the bonded wafer has a period half of that 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.

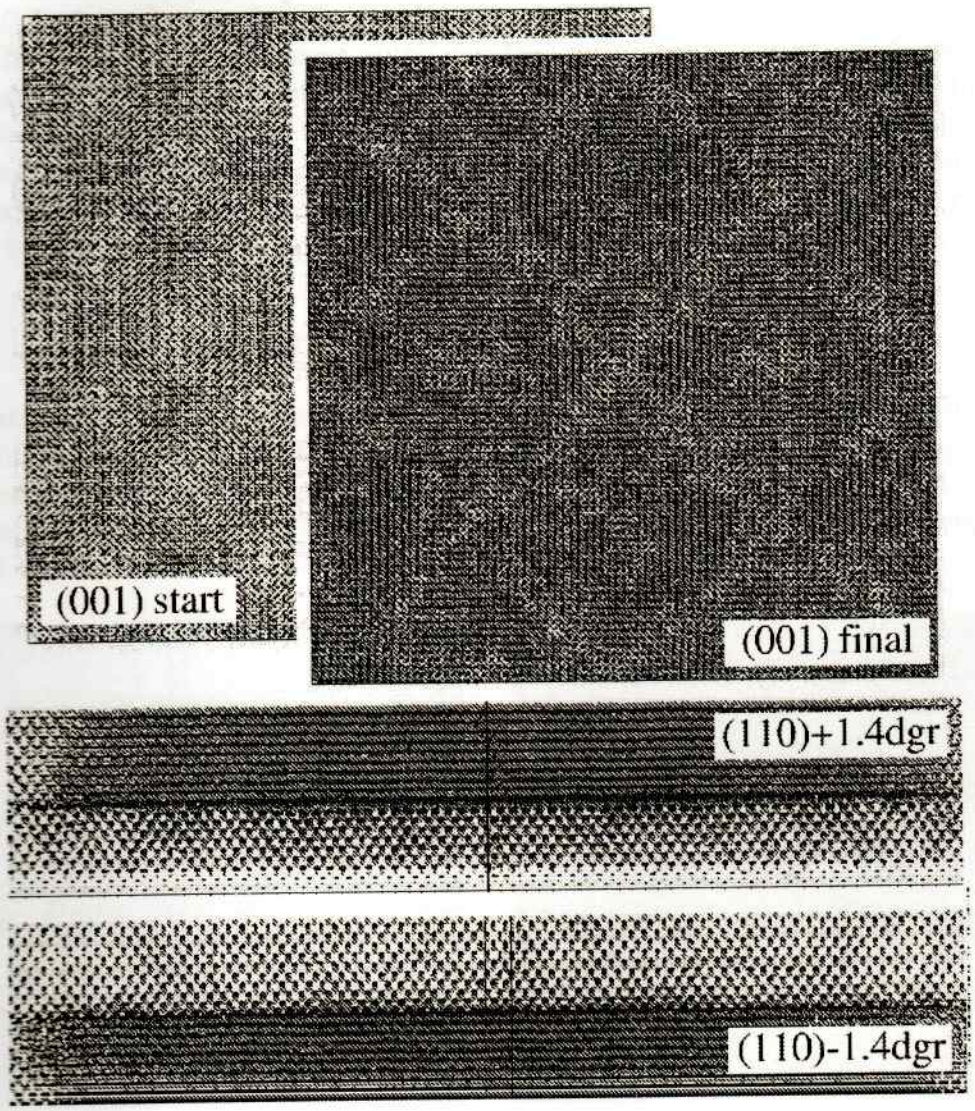


Figure 6: MD simulated structural models ([001] and [110] views) of bonded GaAs wafers with a rotationally twist angle of 2.8° annealed at 600K for parallel dimer start configurations (134500 atoms, 22x22x6 nm box, 10000 atoms fixed).

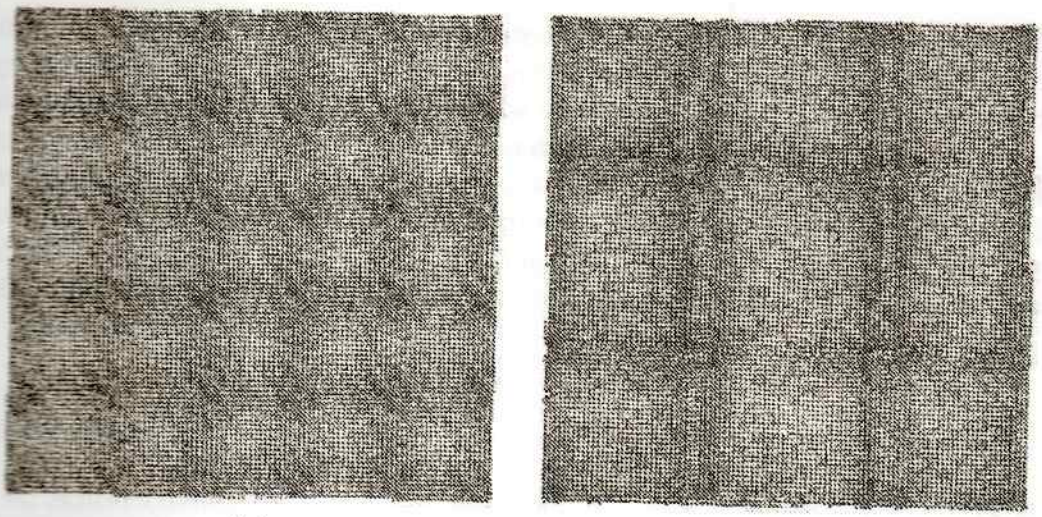
Whereas all simulations shown in Fig. 4 with parallel dimerization at start clearly demonstrate the creation of the screw dislocation network, for orthogonal dimerization or small twist angles this is no longer valid. In Fig. 5 bonding with orthogonal start configurations (a,b) are compared with parallel dimer start configuration (c,d). Thus the bonding of Figs. 5 (a,b) may be considered as bonding with an additional 90° twist rotation. Clearly the periodicity of the defect region is twice of those of (b,c) smoothing out the interface, but creating additional shear strains. Independently from the chosen twist angles and box dimensions all final structures yield bond energies of

approximately $4.5eV/atom$ at $0K$, however, varying slightly with the twist angle. A maximum occurs between 4^o and 6^o twist related to a change of the bonding behaviour itself. As higher the annealing temperature as better the screw formation.

The MD simulation of wafer bonding in the system GaAs/GaAs is presented in Figs. 6 for the same parameter configuration as used for Figs. 4 (b). The parametrization of the Tersoff potential seems to be valid for this system as well as for Si/Si and Si/SiGe etc. The rearrangement of the interface region yields clearly separated screw dislocations as can be revealed comparing start and relaxed atomic projections in [001] direction as well as looking along the [110]-screw dislocations. Besides the dislocation core regions and the transition layers around the interface, the unrotated wafers have approximately the start orientation far from the interface (cf. the slightly rotated views by $+1.4^o$ and -1.4^o around [110]).

Twist wafer bonding of very thin layers

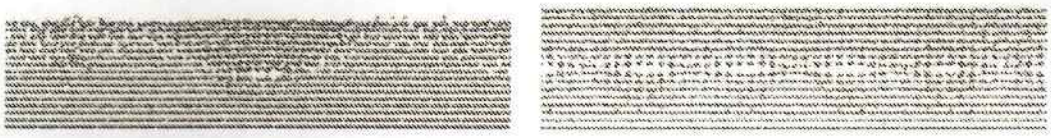
In contrast to the simulations of the bonding process of two bulk wafers presented in the preceeding chapter, the MD simulation of bonding thin wafers yields rippling at the free surfaces, not compensated by the avalanche effect of widely extended crystal lattices. Two wafers of 8 atomic layers thickness are taken, one of them having the lowest layer fixed to approximate the continuation into a large bulk.



(a) (b)

Figure 7: Typical nodes of [110]- and [$\bar{1}$10]-screw dislocations in [001] view after relaxation (b) of the initial (a) 2.8° twist bonded interface resulting from MD simulated bonding of thin wafers.

The Figure 7 demonstrate the wafer bonding of a very thin slice on top of a bulk support with a twist of 3°. Depending on the chosen rotational twist the plan views of the initial configurations (cf. Fig. 7(a)) and the MD relaxed model (cf. Fig. 7(b)) reveal Moiré patterns and screw dislocation networks with varying periodicity, respectively. The Moiré pattern derives from the wafer periodicity projected onto the [001] plane, while the screw dislocation network, having twice the Moiré pattern periodicity, derives from the structural periodicity at the interface. The cross section in [110]



(a) (b)

Figure 8: Interfaces after MD-relaxation of thin bonded wafers with 2.8° (a) and 12.7° twist (b) in [110] projection showing the different defect core structures.

projection, i.e. along the dislocation lines as shown in Fig. 8 for enlarged selections of bonded 2.8° (a) and 12.7° (b) twist boundaries, illustrate both, the perfect bonding in areas between the dislocations, and a rippling of the free surfaces of the thin layer. The rippling effect, not observed on thick wafers, are due to the possibility to bend the thin layer: Along the screw dislocations the bonding distance between the wafer increases slightly, indicating varying strains within the wafer. This results in an additional displacement of the atomic planes close to the screw dislocation, which for thin wafers continue towards the surface. It diminishes with increasing distance from the interface and will thus vanish for increasing thickness of the bonded wafers.

Conclusions

Molecular dynamics simulations (MD) based on empirical potentials are used to investigate the bonding of two Si(001) wafers rotationally misaligned. Calculated bonding energies and forces strongly depend on the initial twist and result in special interface configurations no longer perfectly coordinated. 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. In addition, thin wafers have been simulated. Unlike bonding bulk wafers, the MD simulations for thin wafers yield effects at the free surfaces, like welding and straining, not compensated by the avalanche effect.

References

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