A model for shear mechanism in the pyroxene-ilmenite transition in MgSiO$_3$

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1. Introduction

Phase transition mechanisms of silicate minerals under high-pressure play significant roles to the rheological properties and transformation kinetics in the Earth's mantle. To understand the dynamics of the Earth's interior, previously, many researchers have studied the transformation mechanisms of olivine to wadsleyite (beta-phase) or ringwoodite (gamma-phase). In addition to the nucleation and growth mechanism, Poirier (1981) first proposed a shear-promoted mechanism for the olivine-ringwoodite transition in Mg$_2$SiO$_4$. This diffusionless mechanism forms coherent lamellar intergrowths of product high-pressure phases in the host minerals. Pyroxene is the second major constituent of the upper mantle. However, there is no direct experimental work for the transition mechanism of MgSiO$_3$-rich pyroxene under high pressure. In this study, it is intended to propose a model of shear mechanism for the MgSiO$_3$ clinoenstatite to akimotoite (ilmenite phase) transition based on natural occurrence of enstatite and akimotoite and the topological perspective on both the structures.

2. Clinoenstatite-akimotoite intergrowth in a shocked meteorite

Lamellar intergrowth of akimotoite (MgSiO$_3$-ilmenite) with clinoenstatite (S.G. $P2_1/c$) was identified in the heavily shocked meteorite Tenham. Akimotoite shows lamellar intergrowth and a topotaxial relationship with host clinoenstatite (Tomioka & Fujino 1999) (Fig.1). These planes correspond to the layers of the nearly close-packed oxygen for both structures (Fig.2). Enstatite associating with akimotoite is low temperature clinoenstatite ($P2_1/c$). According to high-pressure experiments of MgSiO$_3$, High-pressure clinoenstatite ($C2/c$) is stable above ~7 GPa (Angel et al. 1992). This phase cannot be recovered to the ambient condition, but inverted into $P2_1/c$ phase. Hence, $P2_1/c$ clinoenstatite in Tenham could be an inversion product of high-pressure clinoenstatite ($C2/c$) during the pressure release in shock event. Akimotoite would have formed from the host orthoenstatite ($Pbca$) via $C2/c$ clinoenstatite.

Fig.1 Intergrowth of akimotoite with clinoenstatite. (a) Electron micrograph. (b) SAED pattern taken from the area including both clinoenstatite and akimotoite in (*a*). This pattern shows a nearly topotaxial relationship: (0001)$_{Ak}$ is parallel to (100)$_{Cen}$

Fig.2 Relationship of crystallographic orientations between MgSiO$_3$ clinoenstatite and akimotoite. Schematic drawings represent the close-packed layers of oxygen ions for clinoenstatite (upper left), akimotoite (upper right) and their superimposition (bottom left), respectively.

(100)$_{Cen}$ // (0001)$_{Ak}$

(010)$_{Cen}$ // (10$\overline{1}$0)$_{Ak}$

3. A possible model for shear mechanism in the enstatite-akimotoite transition
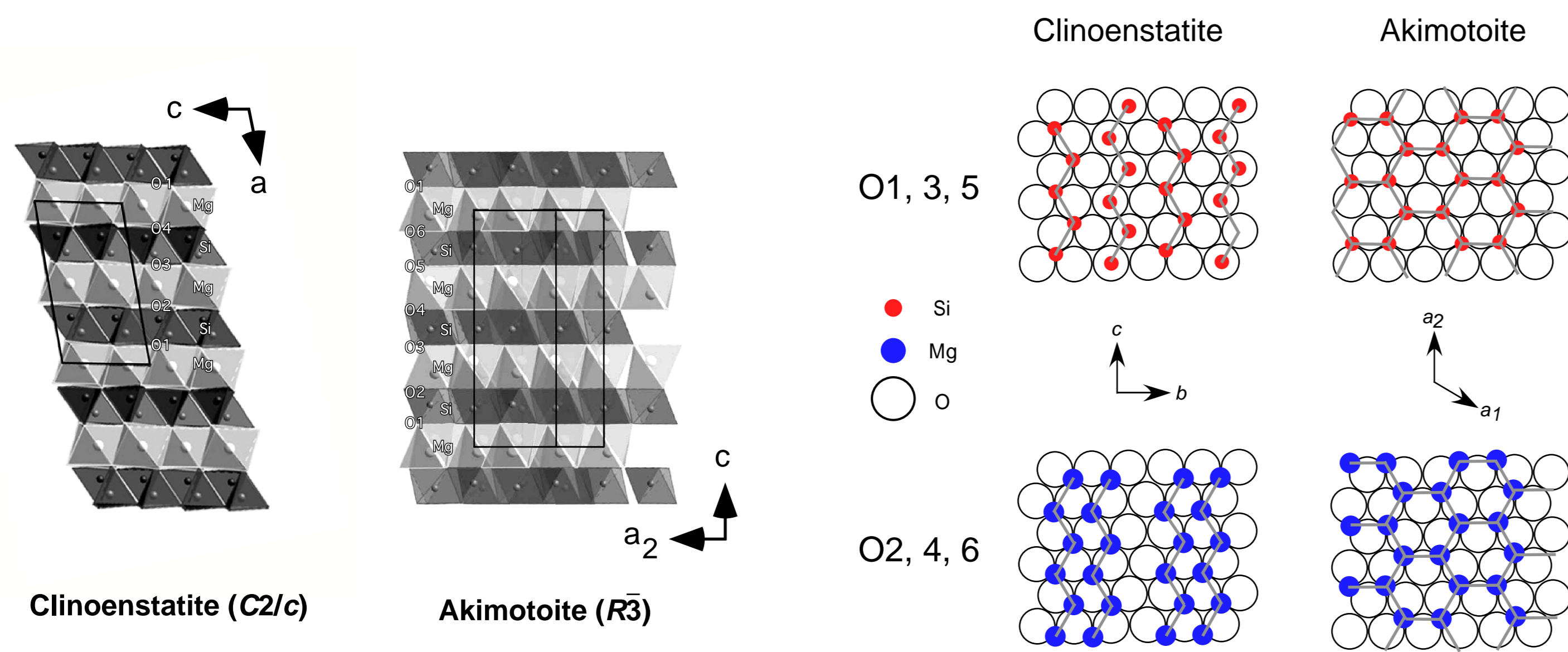

Fig. 3 Crystal structures of clinoenstatite ($C2/c$) and akimotoite ($R\overline{3}$). Both structures are composed of the close packing of oxygen ions: clinoenstatite (ccp); akimotoite (hcp). O1-O6 represent oxygen layers.
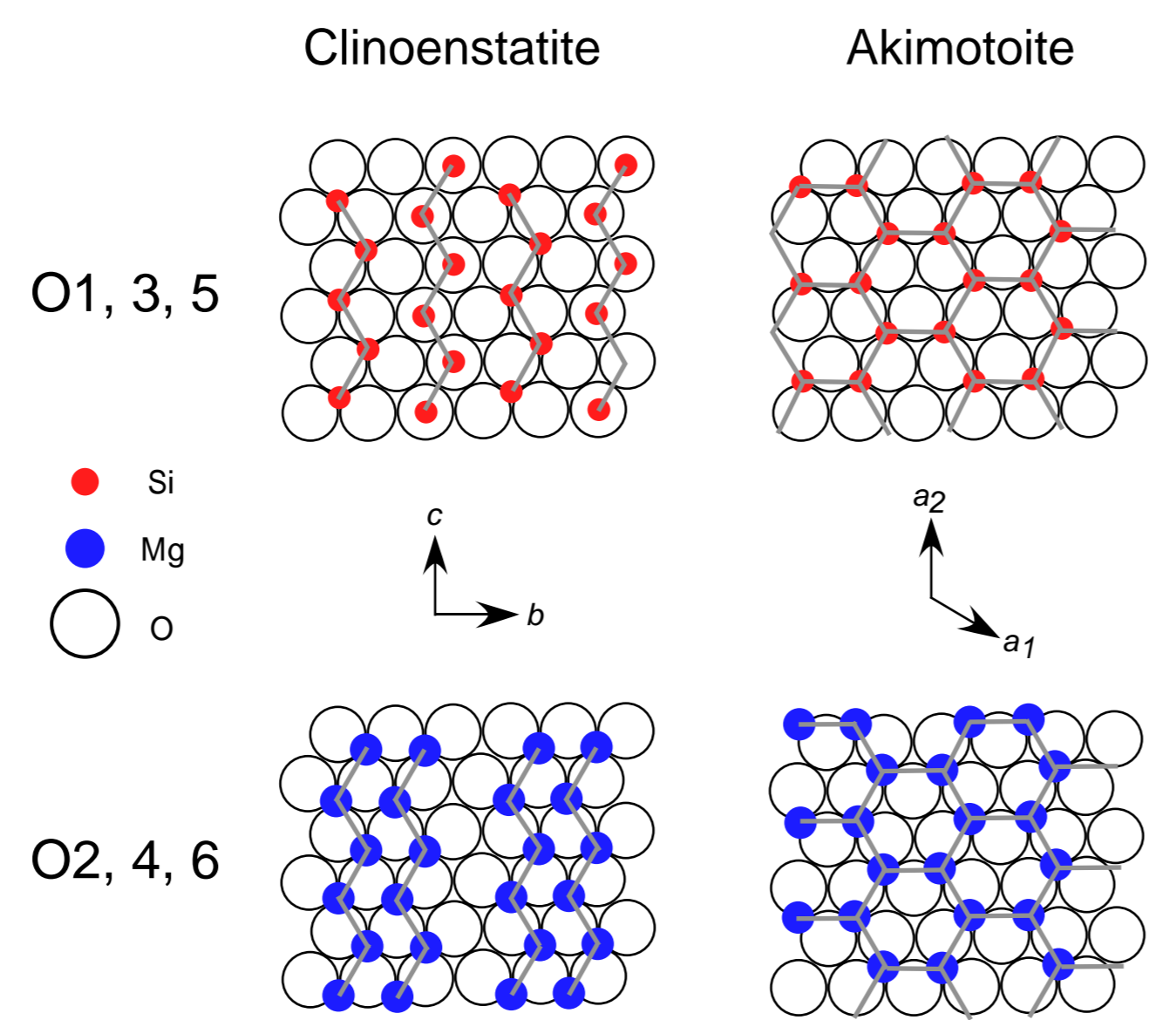
Fig. 4 Simplified packing mode of clinoenstatite ($C2/c$) and akimotoite. O1-O6 correspond to those in fig. 3.

<Oxygen packing>
clinoenstatite ($C2/c$) --- ccp
akimotoite ($R\overline{3}$) --- hcp
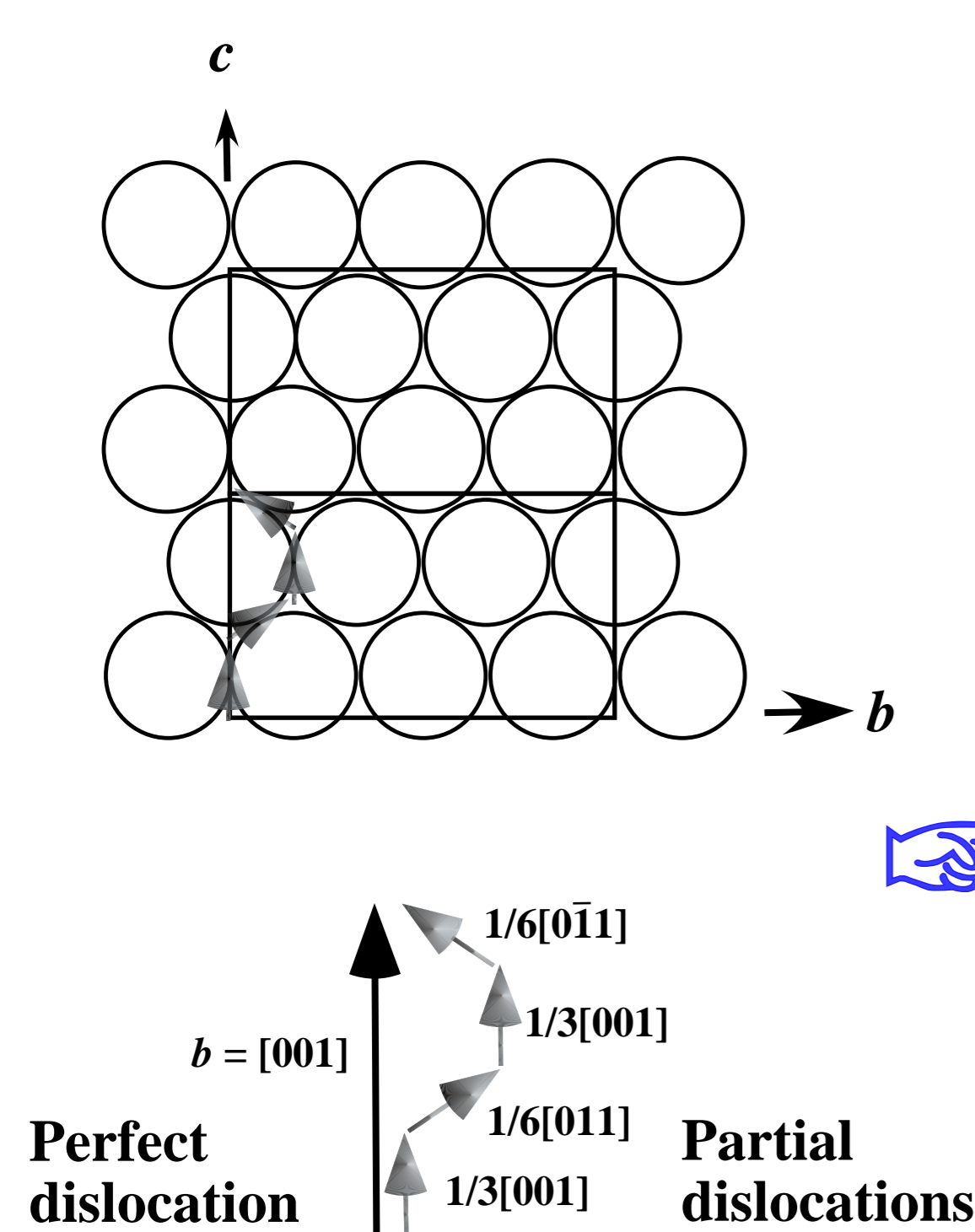The interstices of oxygen layers are filled with Mg and Si ions, alternatively (Fig. 3,4).

Fig.5 Dissociation of dislocation in clinoenstatite. Open circles represent oxygen ions on (100) plane.

The shear of oxygen sublattices can be done by the sweeping of partial dislocations along the close packed plane (100) of clinoenstatite. The vector [001] is the smallest translational vector for clinoenstatite and it can be dissociated into four partials (Fig. 5).
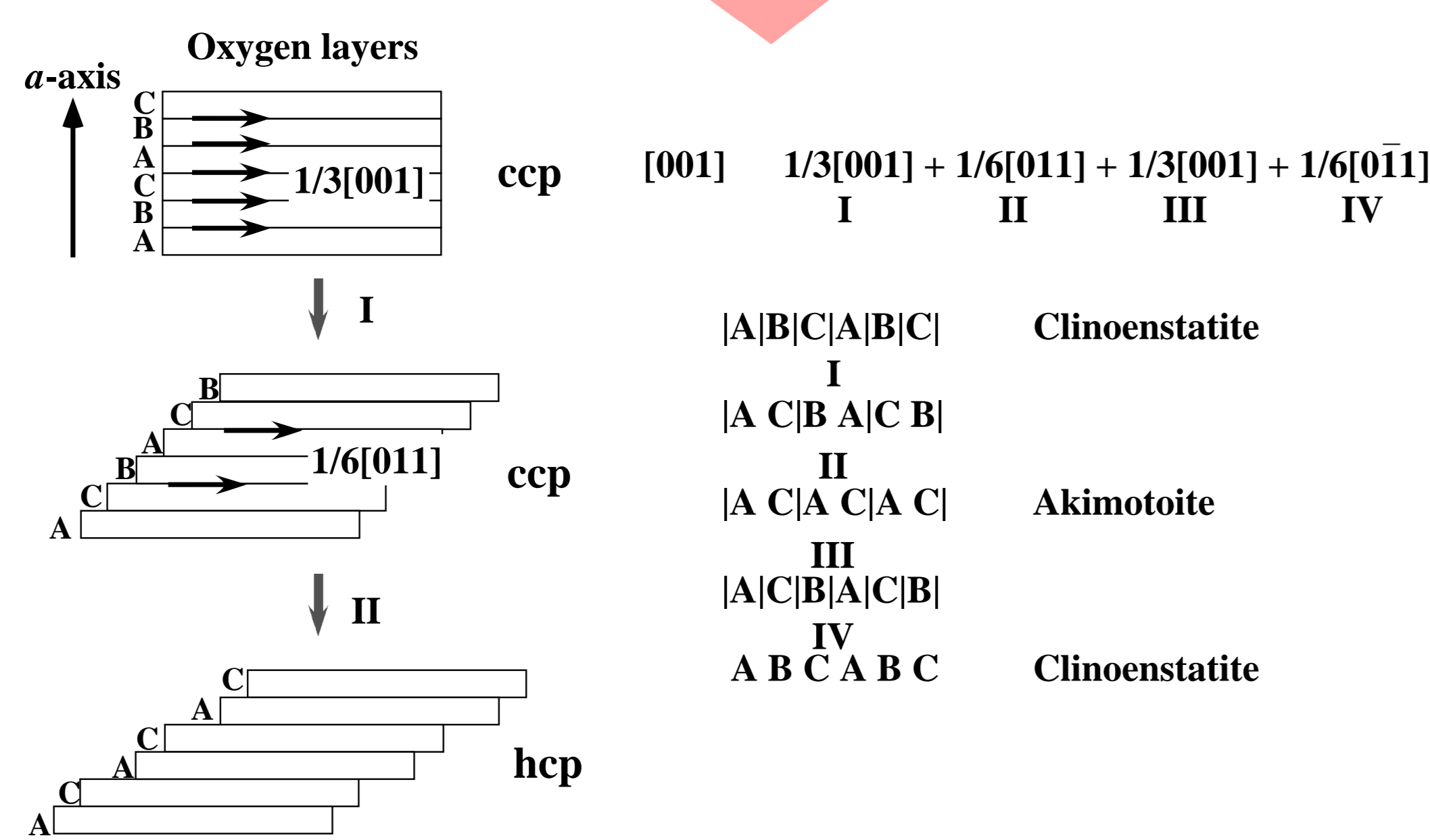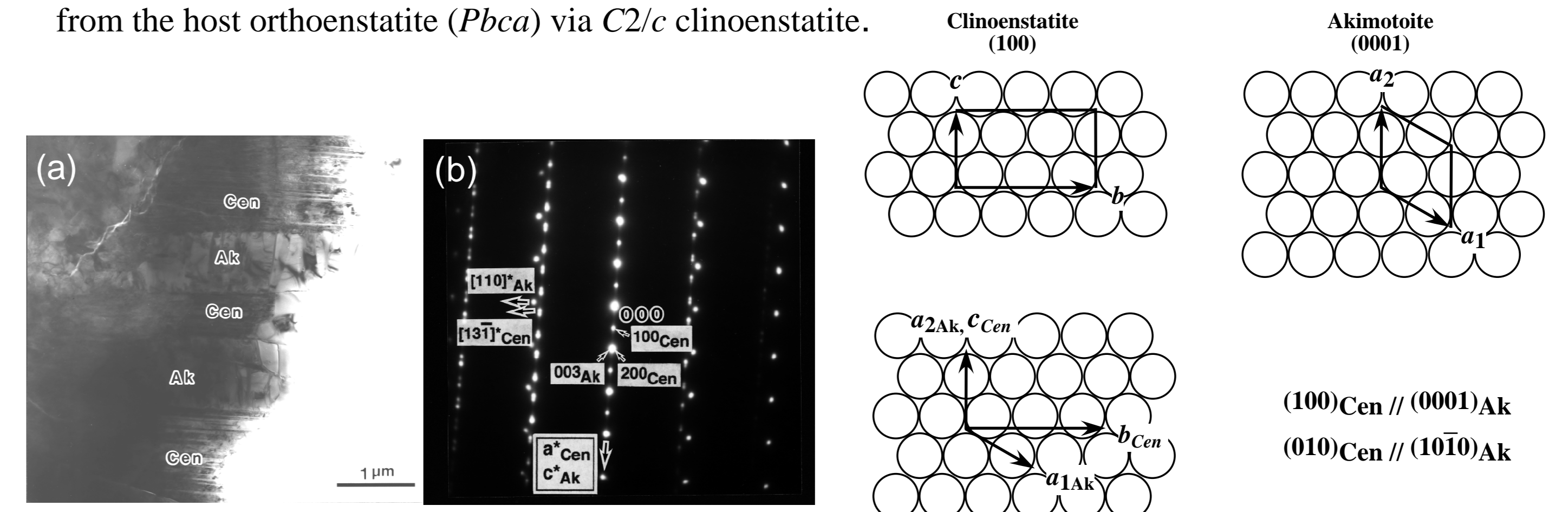

Fig.6 The changes of stacking sequence of oxygen layers in the clinoenstatite-akimotoite transition. The stacking of ccp (clinoenstatite) converts into hcp (akimotoite) by the sweeping of two partial dislocations. The first shear (I) is promoted by a partial dislocation 1/3[00$\overline{1}$] between every oxygen layer. This shear maintains cubic close packing of oxygen. The second shear (II) is promoted by 1/6[011] partial only between oxygen layers with Mg interstitial layers, that converts ccp into hcp.

The sweeping of two partial dislocations with Burgers vectors 1/3[001] and 1/6[011] change ccp of oxygen sublattices into hcp (Fig. 6).
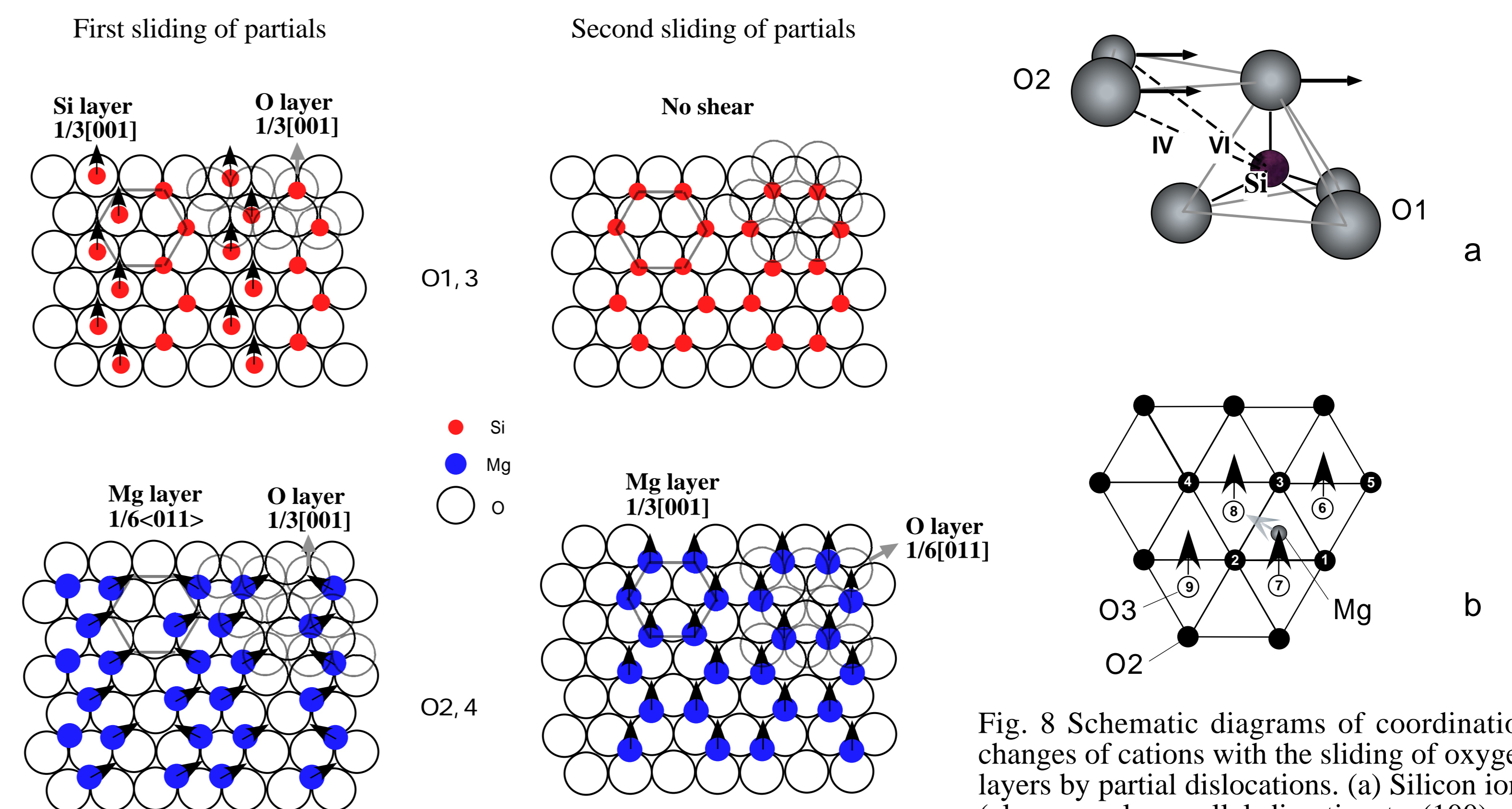

Fig. 7 Synchroshear during the clinoenstatite-akimotoite transition. Gray open circles: oxygen ions in upper layers. Arrows on respective cations indicate the directions of movement associated with the sliding of upper oxygen layers by partial dislocations.
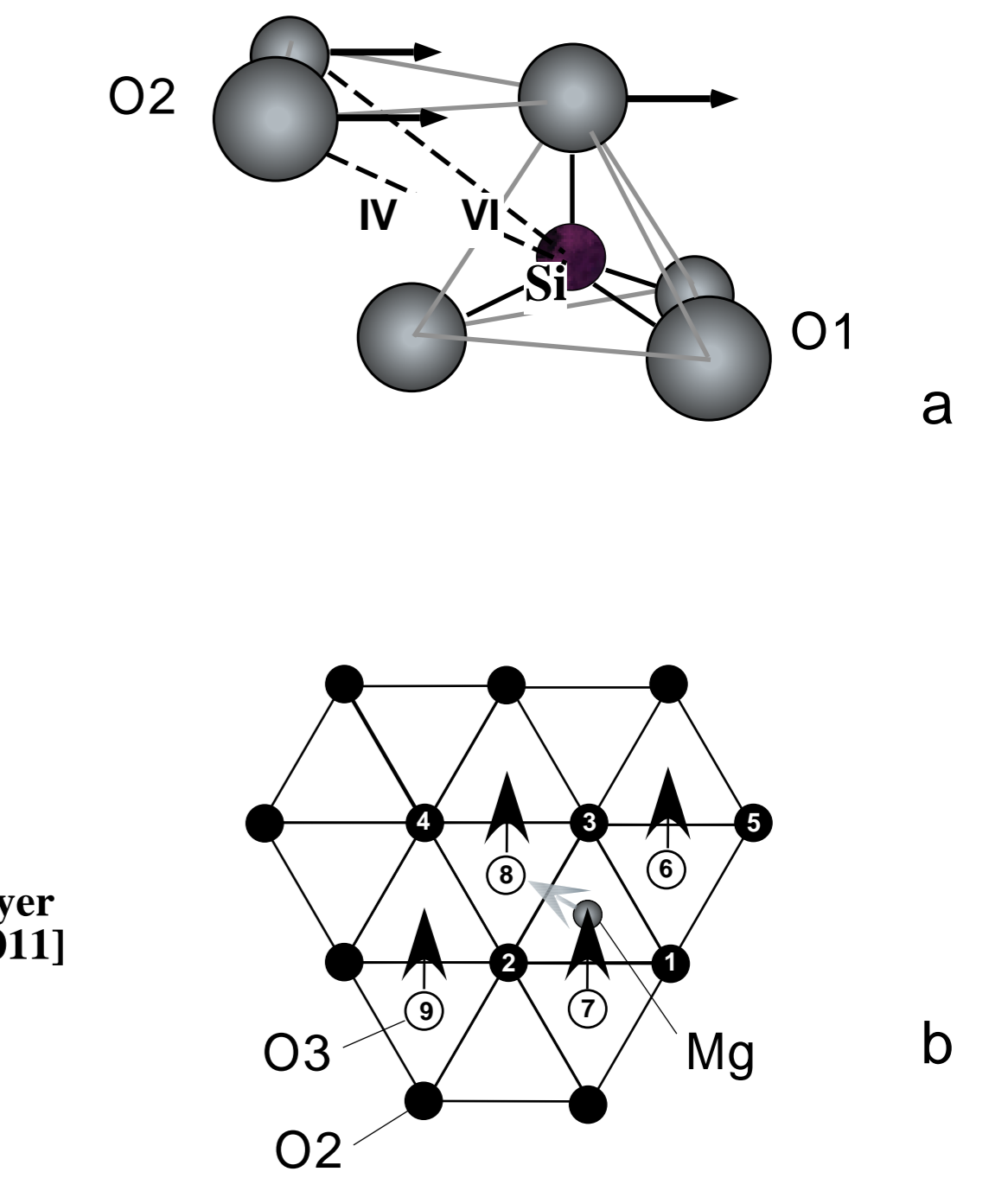

Fig. 8 Schematic diagrams of coordination changes of cations with the sliding of oxygen layers by partial dislocations. (a) Silicon ions (along nearly parallel direction to (100)$_{Cen}$). Solid and broken black lines represent Si-O bonds in the tetrahedral sites and additional Si-O bonds for octahedral sites produced by synchroshear, respectively. (b) Magnesium ions (along the perpendicular direction to (100)$_{Cen}$). Solid arrows represent the displacements of oxygen ions in the upper-oxygen layer. Gray arrow leads magnesium ion to the relocated position of the octahedral site. Mg-O bonds for oxygen ions 1 and 6 are cut, and those for 4 and 9 are re-connected.

Mg and Si ions move cooperatively to the shear of oxygen sublattice (Fig. 7, 8).

This transformation process satisfies the topotaxy as was observed between natural clinoenstatite and akimotoite in the Tenham meteorite (Fig. 2)

4. Summary

1) Two-step shear of oxygen sublattices by the sweeping of the partial dislocations and associating cation shuffling can cause the enstatite-akimotoite transition without any long-range atomic diffusion.

2) This shear mechanism could be more favorable mechanism under high differential stress, or under high pressure but relatively low temperature, where pressure oversteps from the pressure limit of the enstatite stability is large but a long-range atomic diffusion is kinetically hindered.

3) Hogrefe et al. (1994) experimentally demonstrated that the high pressure transitions of enstatite is more sluggish than that of olivine, and suggest that enstatite could directly transform into akimotoite in thick and cold subducting lithospheres. If the shear mechanism in MgSiO$_3$-rich pyroxene is dominant in the subducting slabs, this mechanism drastically enhance the rate of transition from pyroxene to akimotoite. It may cause the deep-focus earthquakes by the transformation faulting due to a rapid and large volume decrease of enstatite in such slabs.

References

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