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► **To cite this version:**

A. Mussi, P. Cordier, D. Mainprice, D.J. Frost. Transmission electron microscopy characterization of dislocations and slip systems in K-lingunite: Implications for the seismic anisotropy of subducted crust. *Physics of the Earth and Planetary Interiors*, 2010, 182 (1-2), pp.50. 10.1016/j.pepi.2010.06.013 . hal-00675799

HAL Id: hal-00675799

<https://hal.science/hal-00675799>

Submitted on 2 Mar 2012

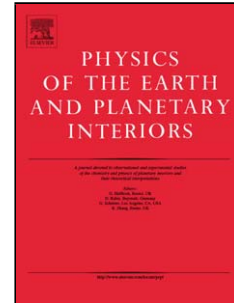
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Accepted Manuscript

Title: Transmission electron microscopy characterization of dislocations and slip systems in K-lingunite: Implications for the seismic anisotropy of subducted crust

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PII: S0031-9201(10)00133-0
DOI: doi:10.1016/j.pepi.2010.06.013
Reference: PEPI 5305

To appear in: *Physics of the Earth and Planetary Interiors*

Received date: 26-3-2010
Revised date: 7-6-2010
Accepted date: 21-6-2010

Please cite this article as: Mussi, A., Cordier, P., Mainprice, D., Frost, D.J., Transmission electron microscopy characterization of dislocations and slip systems in K-lingunite: Implications for the seismic anisotropy of subducted crust, *Physics of the Earth and Planetary Interiors* (2010), doi:10.1016/j.pepi.2010.06.013

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1 **Transmission electron microscopy characterization of dislocations and slip systems in K-**
2 **lingunite: Implications for the seismic anisotropy of subducted crust**

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11
12 **Abstract:**

13 In order to estimate the seismic anisotropy of subducted crust, polycrystalline samples of
14 KAlSi_3O_8 K-lingunite (25% of the total subducted transformed sediments), have been
15 synthesized and deformed under the temperature and pressure conditions of the subducted
16 slabs. Transmission Electron Microscopy (TEM) characterizations of the recovered samples
17 reveal that the microstructures are clearly dominated by [001] glide involving screw
18 dislocations. For this reason, only {100} could be identified as glide planes, the question of
19 [001] slip on {110} remains open. Few $\frac{1}{2}\langle 111 \rangle$ dislocations were observed gliding on {110}
20 planes, which implies that $\frac{1}{2}\langle 111 \rangle\{110\}$ is a harder slip system than those involving [001]
21 slip. The occurrence of sub-grain boundaries suggests that diffusion and climb might be active
22 under these conditions.

23 To assess the texture of polycrystalline K-lingunite, the Crystal Preferred Orientations (CPO)
24 were calculated using Visco-Plastic Self-Consistent (VPSC) polycrystalline plasticity model
25 in simple shear using the slip systems identified by TEM. Finally, the seismic properties of K-

26 lingunite aggregates were calculated from the CPO and single crystal elasticity tensor. K-
27 lingunite is predicted to have a high seismic anisotropy, which could combine constructively
28 with the one of the stishovite (same proportion as K-lingunite at the transition zone depth
29 ranges).

30

31 **Keywords:** K-lingunite, dislocation, slip systems, crystal preferred orientations, seismic
32 properties

33

34 **1. Introduction**

35 The fate of subducted oceanic and continental crust in the mantle is of primary
36 importance for the dynamics of the Earth. It depends largely on the rheological properties of
37 the materials composing the slabs. The high-pressure behaviour of feldspars deserves
38 attention since these minerals are a major component of the continental crust and since they
39 host potassium, an important heat producing radionuclide. At ca. 9 GPa, KAlSi_3O_8 orthoclase
40 transforms to a tetragonal polymorph with a hollandite structure (hereafter referred to as K-
41 lingunite since the hollandite structured $\text{NaAlSi}_3\text{O}_8$ has been previously named lingunite by
42 Liu and El Goresy, (2007). The first synthesis and determination of the crystal structure of K-
43 lingunite ($I4/m$) was conducted by Ringwood et al. (1967). Yagi et al. (1994) and Urakawa et
44 al. (1994) have further investigated its stability using in-situ X-ray diffraction and quench
45 experiments. At higher pressure (ca. 20 GPa), K-lingunite transforms to an unquenchable
46 monoclinic $I2/m$ crystal structure at about 20 GPa (Ferroir et al., 2006). Natural K-lingunite,
47 has been identified in shock veins of heavily deformed ordinary chondrites (Gillet et al., 2000,
48 Tomioka et al. 2000, Xie et al. 2001) and in the SNC achondrite Zagami (Langenhorst and
49 Poirier, 2000a, b). Terrestrial silicate hollandite has also been reported in a strongly shocked

50 anorthosite from the central uplift of the Manicouagan impact crater, Canada (Langenhorst &
51 Dressler (2003)).

52 Assessment of K-lingunite in subducted slabs requires the knowledge of the equation of state
53 and elastic properties of this phase as a function of pressure. Zhang et al. (1993) have
54 determined the compression behaviour of K-lingunite single crystals from ambient pressure
55 up to 4.5 GPa. These results have been extended to higher pressure (15-27 GPa) by
56 Nishiyama et al. (2005). More recently, Mookherjee and Steinle-Neumann (2009) have
57 calculated the elastic properties of K-lingunite up to 100 GPa, based on the density functional
58 theory. To date there is no data of plastic deformation of polycrystals of K-lingunite. However,
59 the single crystal elastic properties cannot be transferred directly to the scale of the
60 polycrystalline aggregate without knowing the Crystal Preferred Orientations (CPO). Plastic
61 deformation by dislocation glide is one of the most efficient mechanisms to generate strong
62 CPO. In this work, Transmission Electron Microscopy (TEM) characterizations of K-
63 lingunite specimens deformed at high pressure are performed to identify the deformation
64 mechanisms of this phase. This information is used to model the CPO and the seismic
65 properties of textured K-lingunite aggregates.

66

67 **2. Material and experimental procedure**

68 *2.1. High-pressure preparation and deformation of the samples*

69 K-lingunite was synthesized from a KAlSi_3O_8 glass in a multianvil press at 17 GPa and at
70 temperatures ranging from 1400 to 1600°C. After synthesis in quasi-hydrostatic conditions,
71 the high-pressure phase was recovered and placed in another high-pressure cell designed to
72 induce deviatoric stresses during the compression (Cordier and Rubie, 2001), at 1300°C, with
73 the same pressure. The deformation conditions corresponding to this second run were 17 GPa,
74 1300°C for one hour (sample 3753) and one hour and a half (sample 2482). In this kind of

75 experiments, large stresses applied during compression are relaxed at high temperature under
76 pressure. After the run, the sample is quenched to ca. 100°C in a few seconds before the slow
77 release of pressure.

78 2.2. Transmission Electron Microscopy

79 Two doubly polished thin foils were obtained from each high-pressure cell. They were
80 thinned to electron transparency with a Gatan® DuoMill™ Model 600 ion milling device and
81 lightly carbon coated. TEM investigations have been performed at a 300 kV accelerating
82 voltage with a Philips® CM30 microscope. As K-lingunite amorphises extremely rapidly
83 under the electron beam damage, a Gatan® cold stage (liquid nitrogen temperature), a small
84 condenser aperture (100 μm) and a small spot size (300 nm), were used in order to preserve
85 the sample long enough to perform the defects characterization. With such an electron
86 illumination, the incident beam current and the fluence rate are respectively 14 nA and
87 $1.2 \times 10^8 \text{ electron.nm}^{-2}.\text{s}^{-1}$, which can be considered as low dose irradiation conditions.

88 The Precession Electron Diffraction (PED) procedure was employed to orientate the grains
89 and to select diffraction vectors. As this technique scans the incident beam in association with
90 a transmitted beam de-scan, at a constant angle throughout the optic axis (Vincent and
91 Midgley, 1994), the spot intensities are reasonably associated with the structure factor and the
92 multiple diffractions are reduced. Indeed, from Morniroli and Ji (2009), the forbidden spots
93 by screw axis and glide plane become very weak for low precession angles and disappear
94 when precession angles reach 3° as in our case. Precession patterns are acquired with the
95 “Spinning Star” device from the Nanomegas® Company. Dislocation Burgers vectors were
96 characterized using the standard extinction conditions ($\mathbf{g} \cdot \mathbf{b} = 0$) as well as with the thickness-
97 fringe method (Ishida et al. 1980, Miyajima and Walte 2009).

98

99 3. Visco-plastic self-consistent model and seismic properties

100 The Visco-Plastic Self-Consistent (VPSC) model has been established in Earth sciences by
 101 Wenk and co-workers (e.g. Wenk et al., 1991) as a model that provides a robust solution for
 102 the CPO development in mineral aggregates deforming by dislocation glide. The model was
 103 originally developed by Molinari et al. (1987) and extended to anisotropic materials by
 104 Lebensohn and Tomé (1993) and a recent review of the method is given by Tomé and
 105 Lebensohn (2004), thus only a short overview is presented in this section. This model has
 106 been successfully applied to many minerals of the Earth's mantle (e.g. olivine, Tommasi et
 107 al., 2000, wadsleyite, Tommasi et al., 2004, stishovite, Cordier et al., 2004).

108 The VPSC model is based on three assumptions: (i) the crystals that constitute the
 109 polycrystal deform uniquely by homogeneous intracrystalline slip, (ii) individual crystals
 110 obey a viscous rheology with shear strain rate proportional to shear stress raised to a power n ,
 111 and (iii) the aggregate behaviour may be calculated as a volume average of the behaviour of
 112 the individual crystals. Locally, from crystal to crystal, stress and strain are heterogeneous and
 113 crystals, in an easy glide orientation, deform faster than those in low resolved shear stress
 114 orientations. Strain compatibility and stress equilibrium are ensured at the macroscopic scale,
 115 i.e. the polycrystalline stress (Σ_{ij}) and strain rate (E_{kl}) tensors are taken to be the volume
 116 average of the stress (σ_{ij}) and of the strain rates (ϵ_{kl}) tensors of the individual component
 117 crystals. The interaction between an individual crystal and a Homogeneous Effective Medium
 118 (HEM) (i.e. the polycrystalline aggregate) is treated using the inclusion formalism of Eshelby
 119 (1957), where each crystal is considered as an ellipsoidal inclusion. Eshelby has shown that
 120 the ellipsoidal inclusion has the unique property of having uniform internal stress, strain and
 121 strain rate fields. The uniform stresses and strain rates of the individual crystals are thus
 122 related to the macroscopic HEM polycrystalline quantities through,

$$123 \quad \epsilon_{kl} - E_{kl} = -\alpha M_{ijkl} (\sigma_{ij} - \Sigma_{ij})$$

124 where M_{ijkl} is the interaction tensor which depends on the rheological properties of the
125 polycrystal and the ellipsoidal shape of the inclusions. The constant α describes the interaction
126 between crystals and the HEM, i.e. it imposes more or less stringent kinematics conditions on
127 crystals. A zero value of α corresponds to the Taylor (1938) model (the upper mechanical
128 bound approach) that imposes a homogeneous strain on all crystals (i.e. $\epsilon_{kl} = E_{kl}$) and requires
129 that at least five independent slip systems are available. A value of one corresponds to the
130 tangent VPSC model of Lebensohn and Tomé (1993), and an infinite value corresponds to the
131 stress equilibrium model (i.e. the lower bound approach; Chastel et al., 1993). The VPSC and
132 stress equilibrium models can operate with less than five independent slip systems, as locally
133 strain compatibility is not required.

134 To perform a calculation model we need to define the initial CPO, the initial crystal shape, the
135 interaction parameter α , the power law stress exponent (n), a constant imposed velocity
136 gradient tensor, a set of slip systems and their relative critical resolved shear stresses. Here we
137 have taken the initial CPO to be composed of 1000 random individual orientations with
138 spherical shape. We have chosen the standard tangent model with $\alpha = 1$ for all simulations.
139 We have no information about the stress exponent for K-lingunite from our experiments and
140 we have assumed a value of 3, which is typical of many minerals at high temperature. The
141 VPSC model is not very sensitive to n , between 3 and 5, and almost all minerals have stress
142 exponents in this range. Increasing n rises the degree of CPO for a given finite strain. In the
143 present models, an aggregate of 1000 random orientations was deformed with a constant
144 velocity gradient tensor for simple shear for 80 identical steps of 0.025 equivalent strain,
145 giving a final equivalent strain of 2.0 (shear strain $\gamma = 3.46$). The slip systems were
146 determined by TEM, but we do not know their Critical Resolved Shear Stresses (CRSS).
147 Based on the dislocation microstructure, we will propose the choice of CRSS.

148

149 **4. Results**

150 *4.1 Dislocation observations and characterisation*

151 The specimen microstructure is heterogeneous. The grain size ranges from 45 to 85 μm and
 152 some are free of dislocations. Nevertheless, most of them contain dislocations generated by
 153 plastic deformation. The density of free dislocations has been estimated of the order of 3.10^{12}
 154 m^{-2} using the method proposed by Ham (1961).

155 *Figure 1.*

156 The samples show pervasive evidence of low-angle sub-grain boundaries (Figure 1). In every
 157 image, the reflecting planes \mathbf{g} and the Zone Axis (ZA) are indicated. Typical dislocation
 158 microstructures of the K-lingunite are shown in Figures 2 and 3. All the images in Figure 2,
 159 are from the same area, but each of them was acquired with different diffracting conditions.
 160 The dislocation population of Figure 2 is composed of two families: dislocations in sub-grain
 161 boundaries as well as free dislocations with $\rho \approx 3.10^{12} \text{ m}^{-2}$. Both families of dislocations are
 162 out of contrast with the diffraction vector $\mathbf{g} = \bar{1}\bar{1}0$ (Figure 2a). Moreover, following the
 163 method of Ishida et al. (1980), the value of the $\mathbf{g}\cdot\mathbf{b}$ product is $n = -1$ with $\mathbf{g} = 4\bar{5}1$ (Figure 2b)
 164 and $n = -1$ with $\mathbf{g} = 0\bar{3}1$ (Figure 2c). The analyses of the number of terminating fringes with
 165 Ishida's method are summarized in table 1. Consequently, the Burgers vector of these
 166 dislocations is $[00\bar{1}]$.

167 *Figure 2.*

168 The dislocations visible in Figure 3 are in contrast with $\mathbf{g} = 2\bar{1}\bar{1}$, with a $\mathbf{g}\cdot\mathbf{b}$ product equal to
 169 $n = -1$ (Figure 3a), and are standing end-on when viewed along $[001]$ (Figure 3b).
 170 Considering other diffraction conditions, the Burgers vector of this family of dislocations is
 171 $[001]$ and they have a screw character. Determining the glide plane of screw dislocations is
 172 difficult; however figure 3b shows many $[001]$ screw dislocations aligned perpendicular to

173 [020] and to [200]. This observation suggests that (010) and (100) may be glide planes for
 174 [001] dislocations.

175 *Figure 3.*

176 Figure 4 shows two populations of dislocations, which exhibit different contrasts and
 177 terminating fringes:

178 - with $\mathbf{g} = \bar{3}01$ (see Figure 4a), the $\mathbf{g}\cdot\mathbf{b}$ product is $n = -1$ for dislocations with the low contrast
 179 (labelled B) and $n = 2$ for the ones with a stronger contrast (labelled A);

180 - with $\mathbf{g} = 00\bar{2}$ (see Figure 4c), the $\mathbf{g}\cdot\mathbf{b}$ product is $n = 2$ for dislocations B and $n = -1$ for
 181 dislocations A;

182 - then with $\mathbf{g} = \bar{2}00$ (see Figure 4b), the $\mathbf{g}\cdot\mathbf{b}$ product is $n = 1$ for dislocations A and
 183 dislocations B are out of contrast.

184 Finally, the Burgers vector of dislocations A is $1/2 [\bar{1}11]$ or $1/2 [\bar{1}\bar{1}1]$ and dislocations B are
 185 of the [001] type. From the orientations observed on figure 4c, the dislocations B have an
 186 edge character. This part of the specimen contains a comparable amount of $1/2\langle 111 \rangle$ and
 187 [001] dislocations.

188 *Figure 4.*

189 Figure 5a shows a curved dislocation segment (circled). The number of terminating fringes
 190 suggests that $n = \pm 2$ $\mathbf{g}\cdot\mathbf{b}$ product with $\mathbf{g} = \bar{2}5\bar{1}$. Considering other diffraction conditions, a
 191 Burgers vector of $\pm 1/2 [11\bar{1}]$ is consistent with all images obtained for this dislocation. The
 192 specimen has been tilted until this dislocation segment appears linear. This is achieved when
 193 the area is observed along the [001] zone axis. The segment appears to lie in the $(\bar{1}10)$ plane
 194 (Figure 5b). Consequently, the slip system of the curved dislocation is $1/2 [11\bar{1}] (\bar{1}10)$.

195 *Figure 5.*

196 Figure 6a shows another curved dislocation for which diffraction experiments give a
197 $\pm 1/2[\bar{1}11]$ Burgers vector. Viewed along the $[001]$ zone axis, this segment appears to lie in
198 the (100) plane (Figure 6b).

199 *Figure 6.*

200 4.2 Visco-plastic self-consistent modelling

201 In order to run the VPSC models we need to define the CRSS for each slip system. The TEM
202 analysis has shown that slip occurs on $[001]\{100\}$, the majority of the dislocations are $[001]$
203 screw dislocations and these could potentially also slip on $\{110\}$ and indeed on all $\{hk0\}$.
204 However, the TEM analysis did not unambiguously identify $\{110\}$ as active slip planes or
205 effectively eliminates them either. As $[001]\{100\}$ dislocations had a high density we have
206 assigned this slip system a low relative CRSS of one. The $[001]\{100\}$ system has probably a
207 CRSS similar to $[001]\{110\}$, we have used a CRSS of one, but also of six to see how the
208 activity of this system affects the CPO. A third slip system is observed, $1/2\langle 111 \rangle\{110\}$, with
209 a lower dislocation density. Without mechanical data, we have assigned a series of CRSS to
210 this slip system between 1 and 6, assuming that it is less frequent because the shear stresses
211 were only high enough to weakly activate the system. Four CRSS models were explored; all
212 had the CRSS for $[001]\{100\}$ equal to one, but the values for $[001]\{110\}$ and $\langle 111 \rangle\{110\}$
213 where either one or six. The results in Figure 7 show for the four CRSS models that the pole
214 figures reveal very little change in the overall distribution and only slight variations of pole
215 figure densities.

216 *Figure 7.*

217 The slip activity associated for the two CRSS models are shown in Figure 8. The $[001]\{100\}$
218 has a high activity (0.4 to 0.8) in all models. The $1/2\langle 111 \rangle\{110\}$ slip system has moderate
219 (0.3 to 0.2) activities in all models even when the CRSS equals six. The $[001]\{110\}$ system

220 has a bi-polar behaviour, if the CRSS equals one it has the same activity as $[001]\{100\}$, if the
221 CRSS equals six, it has virtually zero activity.

222 *Figure 8.*

223 4.3 Seismic properties

224 The high-pressure K-lingunite phase represents between 20 to 30 percent by volume of
225 subducted and transformed argillaceous sediments. The anisotropic seismic properties at
226 mantle pressures can be calculated using the CPO of K-lingunite, presented in Figure 9, and
227 the single crystal elastic constants and pressure derivatives recently predicted, using first-
228 principles by Mookherjee and Steinle-Neumann (2009). The seismic properties were
229 calculated using the numerical methods described by Mainprice (1990; 2007). The properties
230 were calculated at a pressure of 17 GPa, the pressure of the deformation experiments, which
231 is approximately equivalent to a depth of 500 km. At present, no temperature derivatives are
232 available for the elastic constants. In Figure 9, the seismic properties are illustrated using:

- 233 - the P-wave velocity (V_p) in km/s;
- 234 - anisotropy of the difference in velocity between the fastest and slowest shear wave
235 (shear wave splitting), for a given propagation direction and (AVs) as percentage;
- 236 - and the polarization of the fastest shear wave.

237 The main features of the seismic anisotropy are a fast V_p velocity of 11.7 km/s parallel to X
238 and slow V_p velocity of 10.3 km/s parallel to Z. The shear-wave splitting is high in a broad
239 region near the Y direction, normal to X and Z and low near X. The V_p anisotropy is 12.8
240 percent, the AVs anisotropies are 15.1 percent for the CRSS model with all CRSS equal to
241 one, the other models give nearly the same results. The orientation of fastest S-wave
242 polarization is parallel to the XY plane

243 *Figure 9.*

244

245 5. Discussion

246 *5.1 Slip systems and deformation mechanisms*

247 The tetragonal cell of K-lingunite is very anisometric with [001] being much smaller than
 248 [100] or [010] (2.723 Å to be compared with 9.315 Å). From the energetic point of view, it is
 249 expected that [001] dislocations are favoured since their elastic energy (which scales with
 250 μb^2) is about ten times less than those of $\langle 100 \rangle$ dislocations, supposing the $\mu_{[001]\{hk0\}}$ shear
 251 modulus is nearly the same as the $\mu_{\langle 100 \rangle\{0kl\}}$ shear modulus. Our observations support this view
 252 since the large majority of observed dislocations are of the [001] type and no [100] or [010]
 253 dislocations could have been identified. From the crystal structure of K-lingunite, it is
 254 expected that [001] dislocations can glide in {100} or {110}. Most free [001] dislocations
 255 have been shown to be of screw character rendering the identification of the slip planes
 256 difficult. The alignment of dislocations seen along the [001] zone axis suggests that [001]
 257 may have been activated in (010). However, the absence of evidence of [001]{110} glide is
 258 not sufficient to rule out the possibility of this slip system.

259 The body-centered lattice (I) of K-lingunite (I4/m) induces an additional translation vector:
 260 $\frac{1}{2}[111]$. With a 6.726 Å moduli, $\frac{1}{2}\langle 111 \rangle$ dislocations have an elastic energy that corresponds
 261 to six times the one of [001] dislocations, supposing the $\mu_{\frac{1}{2}\langle 111 \rangle\{110\}}$ shear modulus is nearly the
 262 same as the $\mu_{[001]\{100\}}$ shear modulus. The activation of $\frac{1}{2}\langle 111 \rangle$ glide is pervasive in our
 263 samples. The {110} planes have been identified as possible glide planes, in agreement with
 264 crystal structure considerations (Figure 10).

265 *Figure 10.*

266 We have also observed $\pm 1/2[\bar{1}11]$ dislocations aligned along a (100) plane. Since this plane
 267 does not contain the Burgers vector, it must be considered as a climb plane. This is not the
 268 only evidence for climb since we have observed many sub-grain boundaries in several grains
 269 (some well-organized, some less). As already pointed out in previous studies (Cordier and

270 Rubie 2001, Thurel and Cordier 2003), this kind of experiments, where specimens are
271 compressed in a non-hydrostatic environment, correspond to high stresses at the beginning of
272 the heating, which are then relaxed. After a given (unknown) time, the stress level becomes
273 probably very low and recovery processes are enhanced. The large number of subgrain
274 boundaries observed is thus not surprising. However, subgrain formation requires climb (also
275 shown independently with $\frac{1}{2}\langle 111 \rangle$ dislocations) and hence diffusion. Our observations are
276 thus an indication that diffusion is active in K-lingunite at 1300°C.

277 *5.2 Modelling CPO of K-lingunite aggregates and seismic properties*

278 The VPSC models used the slip systems identified by TEM, namely [001] glide (in {100} and
279 possibly in {110}) and $\frac{1}{2}\langle 111 \rangle\{110\}$). The dislocation density of [001] was higher and was
280 dominated by dislocations of the screw character, which could result in “pencil” glide or
281 cross-slip type behaviour on planes in the zone axis of the slip direction [001]. We assigned to
282 this slip system the lowest CRSS of one. Simulations with all the four CRSS show that the
283 CPO has the slip direction [001] parallel to the finite strain extension X direction, and the pole
284 to (100) plane parallel to the finite strain shorting Z axis. In contrast, the $\langle 111 \rangle$ direction and
285 the pole to plane {110} are oblique to Y and Z respectively. The pole figures suggest a
286 dominant activity of [001] glide, which is confirmed by the slip system activity plots. The
287 increase in the CRSS from one to six reduces the activity of the system $\frac{1}{2}\langle 111 \rangle\{110\}$ to
288 about 20%, whereas the same increase for [001]{110} reduces its activity to nearly zero.
289 Reducing the activity of these glide systems is compensated by an increasing activity of
290 [001]{100}. Pole figure densities and symmetries are virtually unaffected by these activity
291 changes because slip in [001] direction is always dominant, either on the {100} plane or a
292 combination of {100} and {110} planes, which will produce pencil-like glide configuration
293 because of tetragonal symmetry of K-lingunite.

294 The seismic anisotropy calculated from the CPO for all CRSS models are also very similar,
295 with:

- 296 - fast V_p parallel to X;
- 297 - the highest shear wave splitting anisotropy parallel to Y;
- 298 - and the fastest S-wave polarization parallel to the XY plane, plane of finite strain
299 shortening normal to Z.

300 At depth of 500 km in the lower part of the transition zone, slabs are often nearly horizontal
301 (e.g. Fukao et al., 2001; Ritsema et al., 2004; Zhao 2004), and are very common in the
302 circum-Pacific region. In such an idealized case, the horizontal propagation direction along X
303 will have a high P-wave velocity and a low S-wave splitting, which would correspond to the
304 down dip direction if the plate is slightly dipping. In contrast, the horizontal propagation
305 direction along Y will have a moderate P-wave velocity and a high S-wave splitting with a
306 polarization of the fastest S-wave being parallel to the horizontal plate (XY) plane. If the plate
307 has slightly dipped, then the polarization would also have a slight inclination in relation to the
308 horizontal. The Y direction would correspond to the transverse direction of the plate, normal
309 to the dip or to the subduction downward transport direction. These results can be compared
310 with the results for stishovite VPSC models reported by Cordier et al. (2004) that we have
311 recalculated at 17 GPa. These results show an almost identical orientation of the seismic
312 pattern:

- 313 - high V_p parallel to X;
- 314 - high shear wave splitting parallel to Y;
- 315 - and the polarization of the fastest S-wave in the XY plane (Figure 9).

316 The anisotropy of V_p and V_s are 13.3% and 7.1% respectively in stishovite. These data can
317 be compared with 12.8% and 15.1% for K-lingunite. Stishovite has a volume fraction of 25%
318 at the transition zone depth ranges. Clearly, the anisotropy of K-lingunite and stishovite

319 would constructively combine giving an effective volume fraction of about 50% of the
320 transformed sediments. The other phases present are majorite (30%), clinopyroxene (5%) and
321 CaAlSi-phase (15%) (Irifune et al., 1994). Of these phases, only majorite is volumetrically
322 important. The pure Mg end-member majorite of the majorite–pyrope garnet solid solution
323 has tetragonal symmetry and is relatively weakly anisotropic with 1.8% for V_p and 9.1% for
324 V_s (Pacalo and Weidner, 1997; Sinogeikin, S.V. and Bass, J.D., 2002a, b). Naturally
325 deformed garnets do not have strong CPOs in eclogites (Mainprice et al., 2004). Nothing is
326 known about majorite CPO, but they are probably similar to the weak CPO of garnets and
327 hence polycrystalline majorite will have isotropic seismic properties. It seems likely that the
328 anisotropic seismic properties of subducted and transformed sediments will be dominated by
329 the combined 50% volume fraction of anisotropic K-lingunite and stishovite.

330 Global studies of radial seismic anisotropy of the deep mantle have shown that in the
331 transition zone (400–700 km depth), regions of subducted slab material are associated with
332 $V_{sv} > V_{sh}$ (e.g. Panning and Romanowicz, 2006; Visser et al., 2008). These global studies
333 would probably not detect the anisotropy associated with a thin veneer of transformed
334 sediments on the slab upper surface. If the anisotropy combined of the K-lingunite and
335 stishovite contributes to the observation of the $V_{sv} > V_{sh}$ signal, then the slab would have an
336 inclination of 45° or more. This aspect seems unlikely for regions with horizontal slabs in the
337 transition zone. However, regional studies of horizontal propagation paths in the mid mantle
338 show that the fastest S-waves are polarized horizontally ($V_{sh} > V_{sv}$) (e.g. Chen and
339 Brudzinski, 2003; Wookey et al., 2002; Wookey and Kendall, 2004). In this case the
340 anisotropy of K-lingunite and stishovite could contribute to this signal, especially if the
341 transformed sediment acted as a wave-guide.

342

343 **6. Conclusion**

344 The plastic deformation mechanisms of K-lingunite are strongly controlled by the plate-
345 shaped crystal structure. The very anisometric tetragonal unit cell strongly favours [001] slip.
346 Most of the dislocations are [001] screws, which makes the determination of glide planes
347 difficult. A secondary slip in $\frac{1}{2}\langle 111 \rangle \{110\}$ has also been characterized with a low
348 occurrence rate. Using the observed glide systems and VPSC model, the CPO of K-lingunite
349 aggregates has been obtained. The texture of polycrystalline K-lingunite shows that the slip
350 direction [001] is parallel to the slab strain X direction and the pole to (100) plane is parallel
351 to the slab strain Z axis. On the contrary, the $\langle 111 \rangle$ direction and the pole to {110} plane are
352 tilted from the Y and the Z slab axes respectively. The seismic properties of K-lingunite
353 aggregates at 17 GPa were calculated according to these CPO and to the single crystal
354 elasticity tensor. Considering that the subducted slab is only composed of K-lingunite, then:

- 355 - The P-waves are faster in parallel with the finite extending X direction (maximal $V_p =$
356 11.7 km/s) and are slower in parallel with the finite shorting Z direction (minimal $V_p =$
357 10.3 km/s);
- 358 - The S-wave anisotropy is characterized by a high shear wave splitting (15.1%) in the
359 finite flattening (XY) plane in the Y direction. The fastest S-waves have their
360 polarization directions in the XY plane.

361 Actually, K-lingunite is 25% by volume of the subducted and transformed argillaceous
362 sediments. The other present phases are stishovite (25%), majorite (30%), CaAlSi-phase
363 (15%) and clinopyroxene (5%). It is expected that majorite has a weak CPO and a weak
364 crystal anisotropy. The seismic anisotropy of the CaAlSi-phase and clinopyroxene phases can
365 be neglected due to their small proportion. Only stishovite is likely to have a strong CPO and
366 a strong single crystal anisotropy. Indeed, stishovite has roughly the same polycrystalline
367 seismic anisotropy pattern than the K-lingunite one, which would combine constructively.
368 Even if the transformed sediments correspond to a thin crustal layer of a thickness of few

369 kilometres, they could act as an anisotropic wave-guide for seismic waves propagating
370 through the slab surface. At a 500 km depth, corresponding to the 17 GPa of the experiments,
371 slabs are often horizontal; hence horizontally propagating seismic waves could sample the
372 transformed sediment anisotropy over long distances.

373

374 **Acknowledgements**

375 We thank H. Schulze for his support of preparation of the thin sections of the recovered
376 samples. The TEM national facility in Lille is supported by the CNRS (INSU) and the Conseil
377 Régional du Nord – Pas de Calais, France.

378

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503 **Table**

504 Table 1 Reflecting planes \mathbf{g} and $\mathbf{g}\cdot\mathbf{b}$ product with Ishida's method.

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505 **Figures captions**

- 506 Figure 1 Micrograph of sample 2482 in WBDF (Weak Beam Dark Field) condition ($\mathbf{g} =$
507 $0\bar{3}1$), along the $[113]$ ZA. Four families of dislocations can be distinguished: \pm
508 $[001]$ dislocations in sub-grain boundaries, $\pm [001]$ free dislocations, $\frac{1}{2}\langle 111 \rangle$
509 dislocations in sub-grain boundaries and $\frac{1}{2}\langle 111 \rangle$ free dislocations.
- 510 Figure 2 Micrographs of sample 2482 in WBDF conditions showing only $[00\bar{1}]$
511 dislocations with two examples of determination of $n = \mathbf{g}\cdot\mathbf{b}$ using the thickness
512 fringes method. (a) Condition $\mathbf{g} = \bar{1}\bar{1}0$, along the $[\bar{1}1\bar{9}]$ ZA; (b) condition $\mathbf{g} =$
513 $4\bar{5}1$, along the $[\bar{1}1\bar{9}]$ ZA; (c) condition $\mathbf{g} = 0\bar{3}1$, along the $[1515]$ ZA.
- 514 Figure 3 WBDF pictures of sample 3753 obtained with $\mathbf{g} = 2\bar{1}\bar{1}$, along the $[315]$ ZA
515 (a) and $\mathbf{g} = 020$, along the $[001]$ ZA (b). These micrographs show numerous
516 $[00\bar{1}]$ dislocations with one example of determination of $n = \mathbf{g}\cdot\mathbf{b}$ using the
517 thickness fringes method.
- 518 Figure 4 WBDF images of sample 2482 with $\mathbf{g} = \bar{3}01$, along the $[010]$ ZA (a); $\mathbf{g} =$
519 $\bar{2}00$, along the $[010]$ ZA (b) and $\mathbf{g} = 00\bar{2}$, along the $[010]$ ZA (c).
520 Micrographs revealing $\frac{1}{2}[\bar{1}11]$ or $\frac{1}{2}[\bar{1}\bar{1}1]$ dislocations and $[00\bar{1}]$ edge
521 dislocations; with five examples of determination of $n = \mathbf{g}\cdot\mathbf{b}$ using the thickness
522 fringes method.
- 523 Figure 5 WBDF images of sample 3753 showing a curved dislocation along the $[1\bar{1}\bar{7}]$
524 ZA, with $\mathbf{g} = \bar{2}5\bar{1}$ (a) and the glide plane along the $[001]$ ZA, with $\mathbf{g} = 0\bar{2}0$
525 (b).
- 526 Figure 6 WBDF images of sample 3753 showing a curved dislocation along the $[001]$
527 ZA, with $\mathbf{g} = \bar{2}00$ (a) and the climb plane along the $[315]$ ZA, with $\mathbf{g} = 1\bar{3}0$
528 (b).

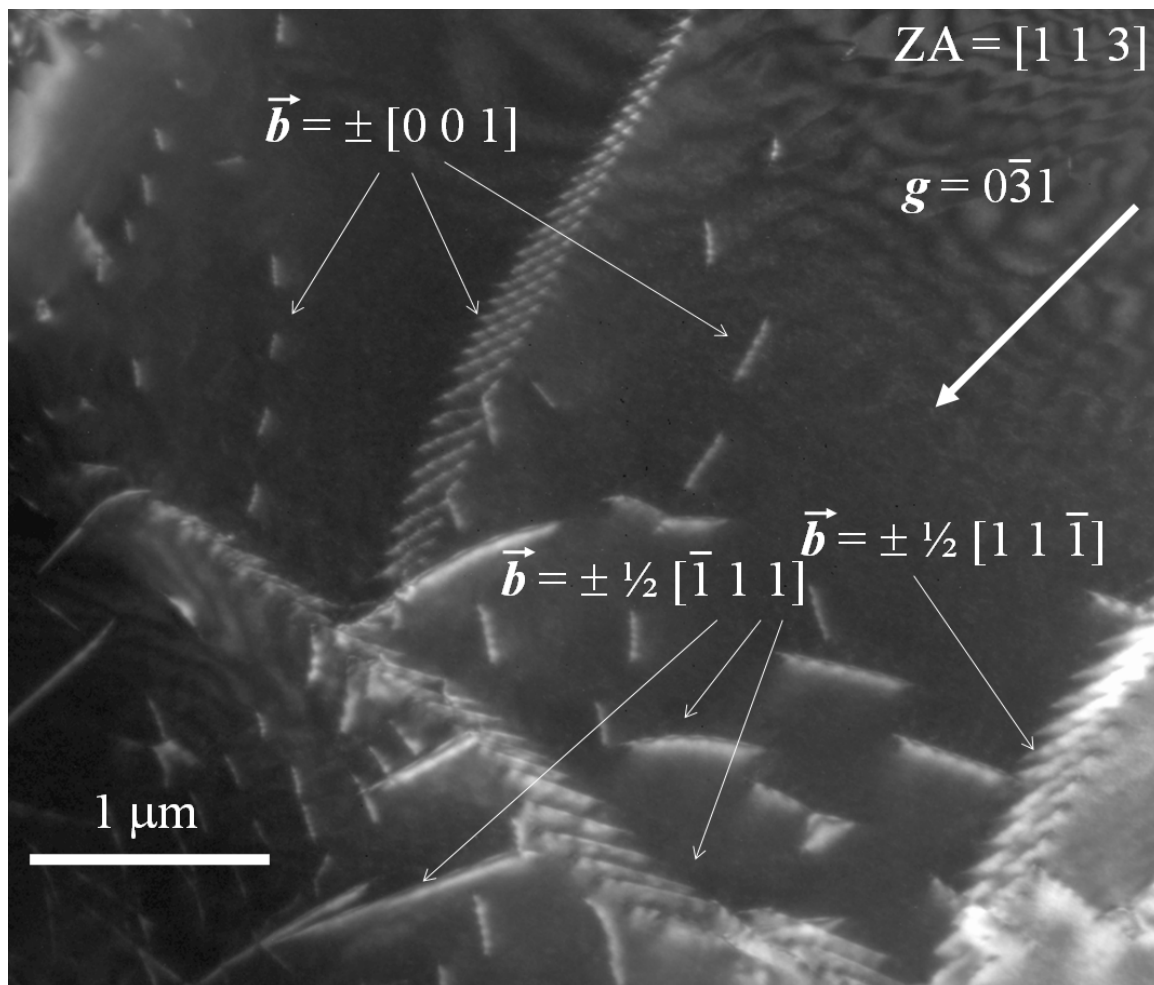
529 Figure 7 Crystal preferred orientation of K-lingunite in simple shear. Model CRSS are
530 marked on the figures. Shear strain (γ) is 1.73 (Von Mises equivalent strain of
531 1.0). Maximum and minimum finite strain axes are marked X and Z. The
532 horizontal black line is the XY flattening plane or foliation. Thick black arrows
533 mark the dextral shear sense, SD is the shear direction and the inclined red line
534 is the shear plane. Lower hemisphere equal area projection.

535 Figure 8 Polycrystalline plastic anisotropy indicated by the slip systems activity as a
536 function of model CRSS in simple shear with $[001]\{100\}$, $[001]\{110\}$ and
537 $\langle 111 \rangle\{110\}$ slip systems. Model A: all slip systems have the same CRSS,
538 corresponding to an isotropic plastic model. Model B: this model has a CRSS
539 of $\langle 111 \rangle\{110\}$ six times greater than $[001]\{100\}$ and $[001]\{110\}$. Model C: it
540 has a CRSS of $[001]\{110\}$ six times greater than $[001]\{100\}$ and $\langle 111 \rangle\{110\}$.
541 Model D: it has a CRSS of $[001]\{110\}$ and $\langle 111 \rangle\{110\}$ six times greater than
542 $[001]\{100\}$.

543 Figure 9 The predicted seismic anisotropy at the pressure of 17 GPa, which corresponds
544 to a 500 km depth. Above: it is composed of 100% polycrystalline K-lingunite
545 with the CPO given in [Figure 7](#) at shear strain of 1.73 for the horizontal flow
546 (XY horizontal plane). The single crystal elastic constants given by
547 Mookherjee and Steinle-Neumann (2009) have been used. Below: it is
548 composed of 100% polycrystalline stishovite with the CPO given in Cordier et
549 al.2004. Horizontal flow (XY horizontal plane). X, Y and Z are the principle
550 finite strain axes where $X > Y > Z$. The black horizontal line is the XY plane of
551 finite strain. Lower hemisphere equal area projection.

552 Figure 10 Projection of the K-lingunite crystal structure along the $[001]$ direction, on the
553 left, and along the $[111]$ direction, on the right (K is symbolized by dark grey
554 spheres, Al octahedral and Si octahedral units are bright grey, with oxygen
555 atom in black). The (100) , (010) , (110) and $(1\bar{1}0)$ glide planes are
556 represented.
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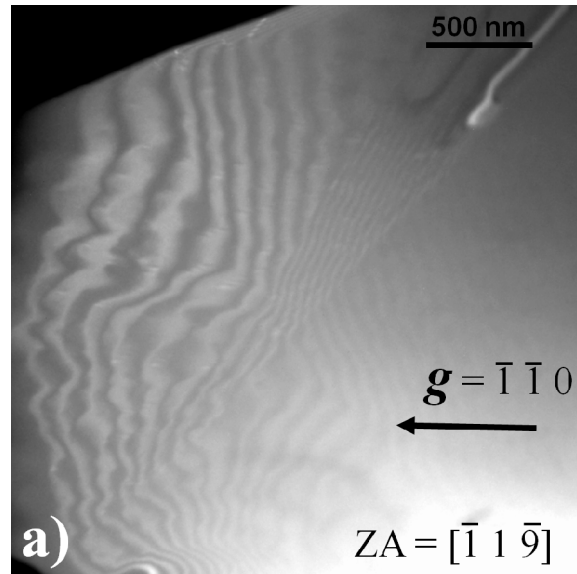
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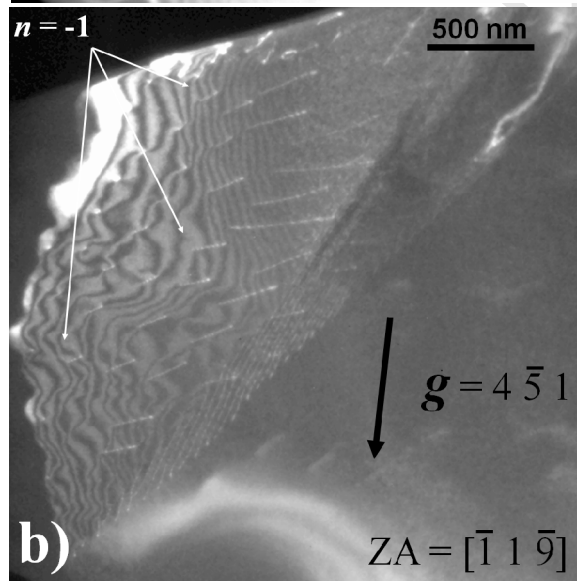
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Figure 1.

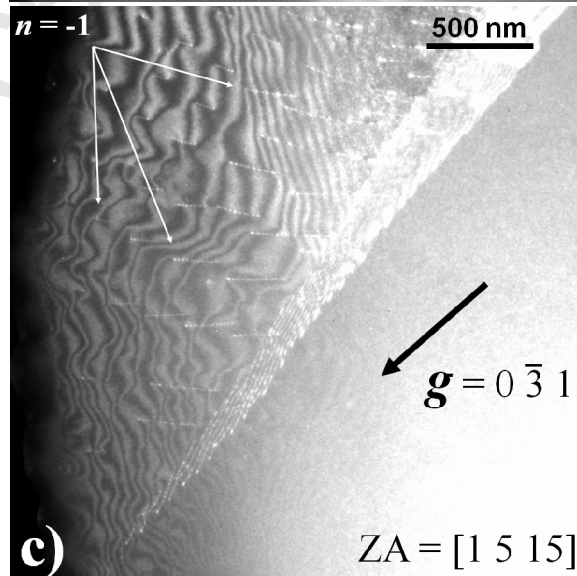
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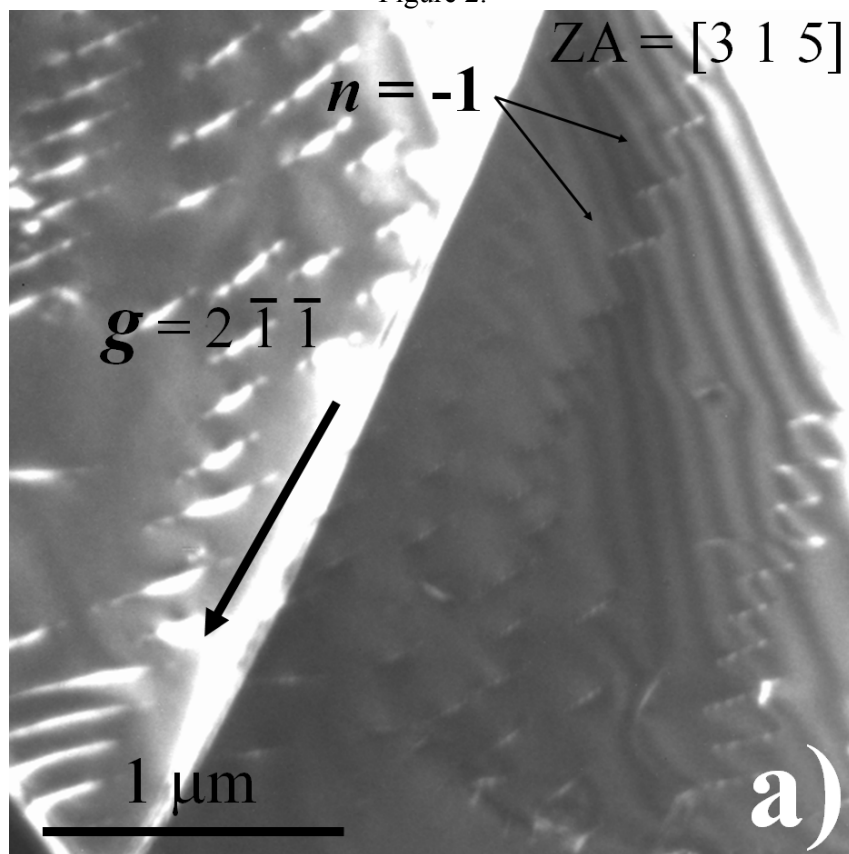


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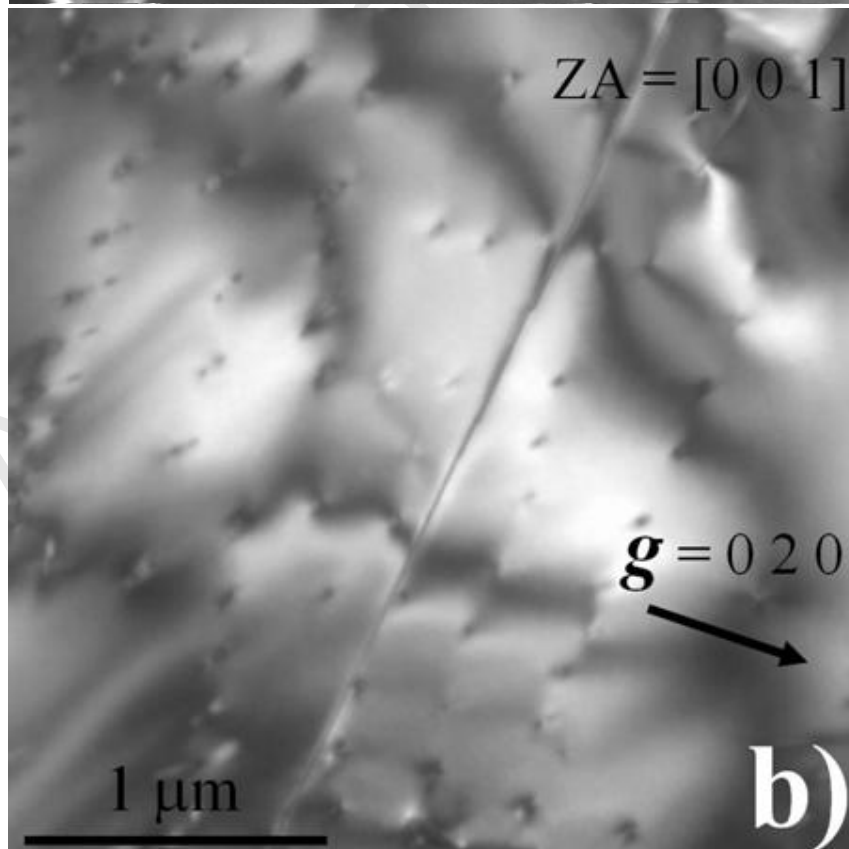


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Figure 2.



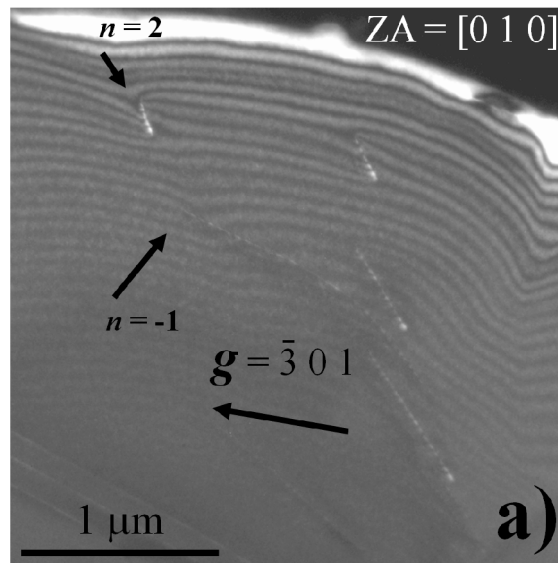
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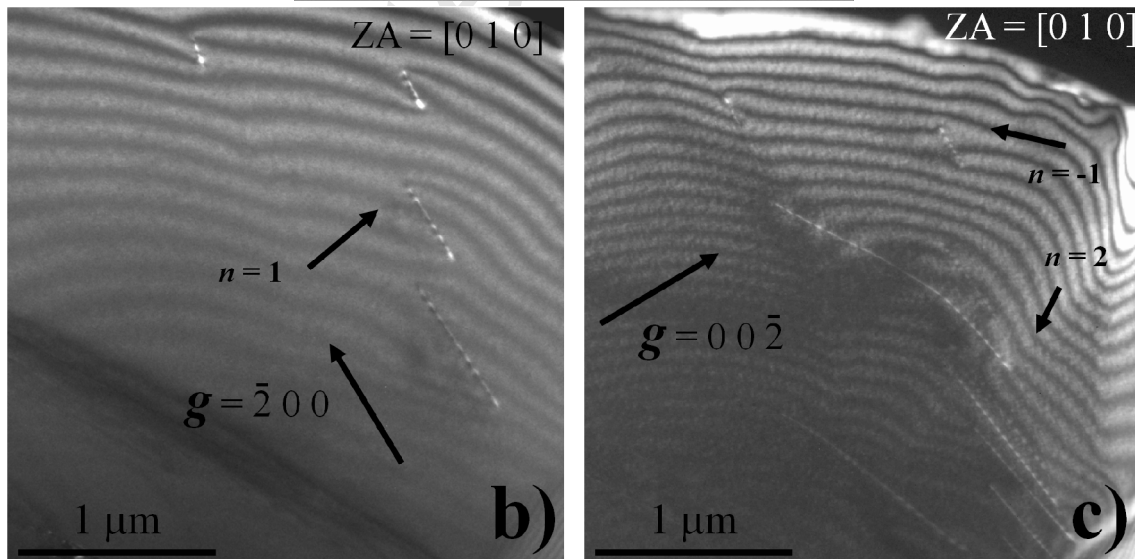
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Figure 3.

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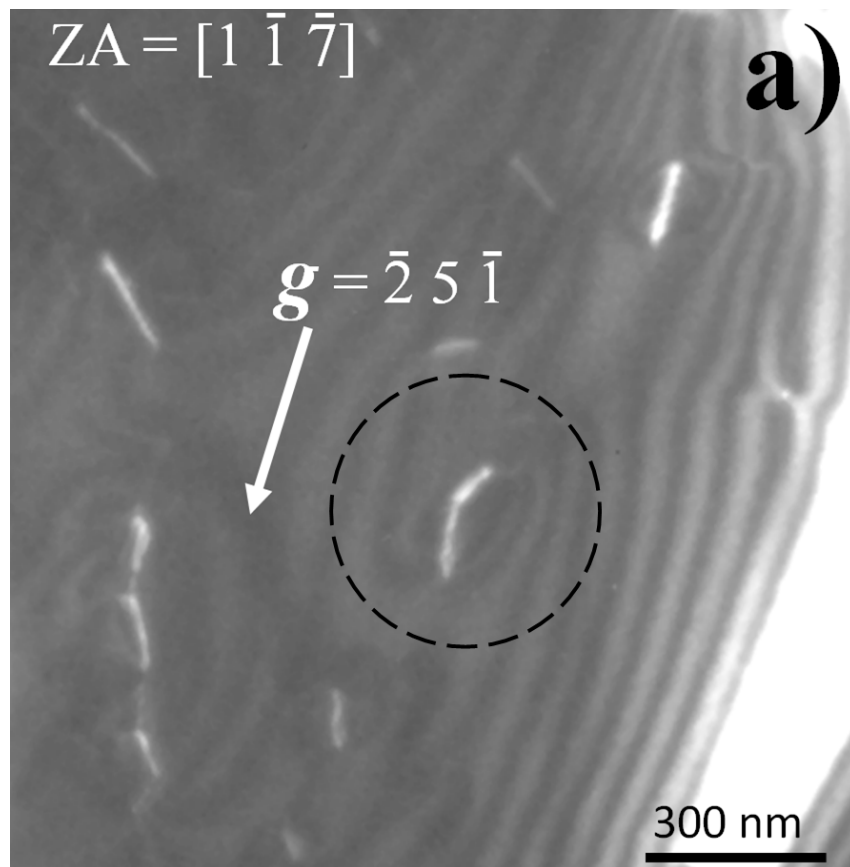
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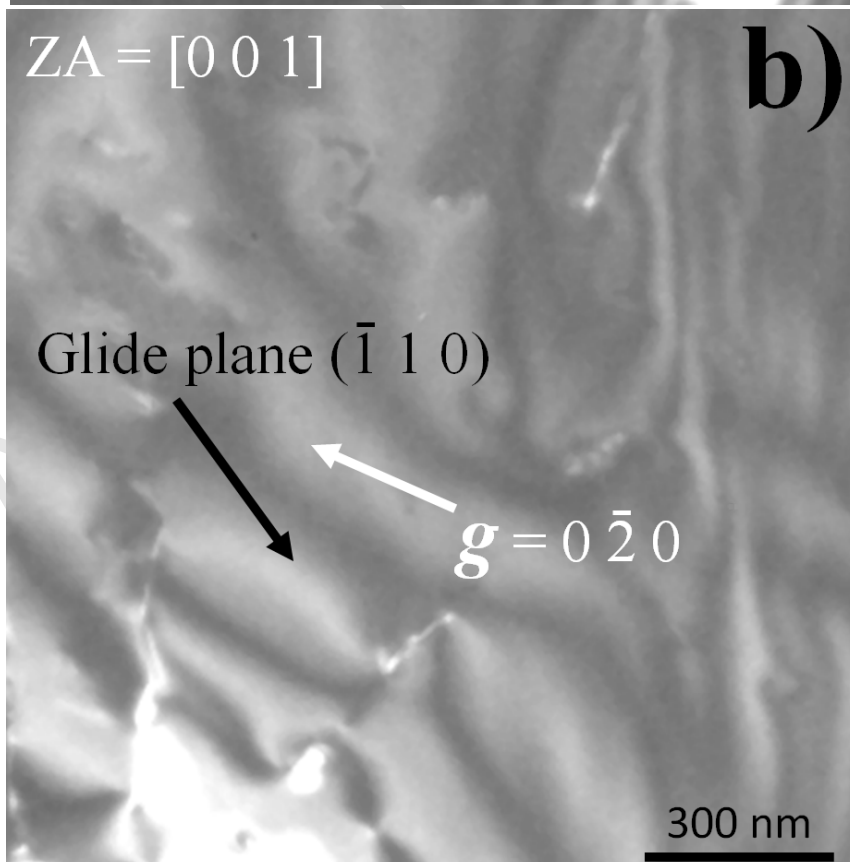
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Figure 4.

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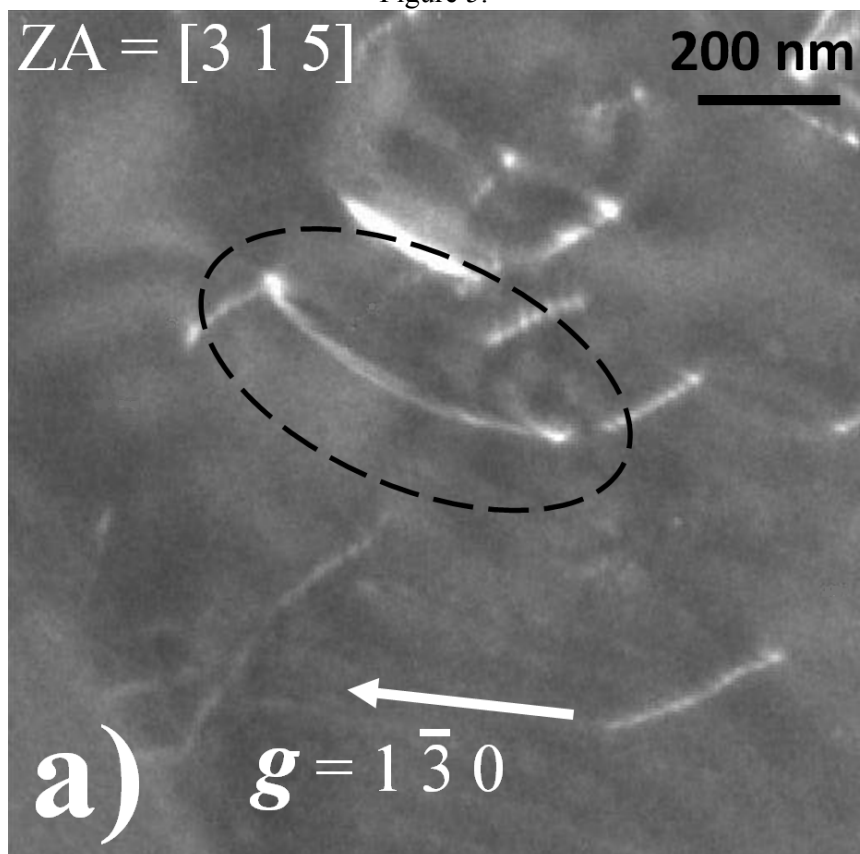
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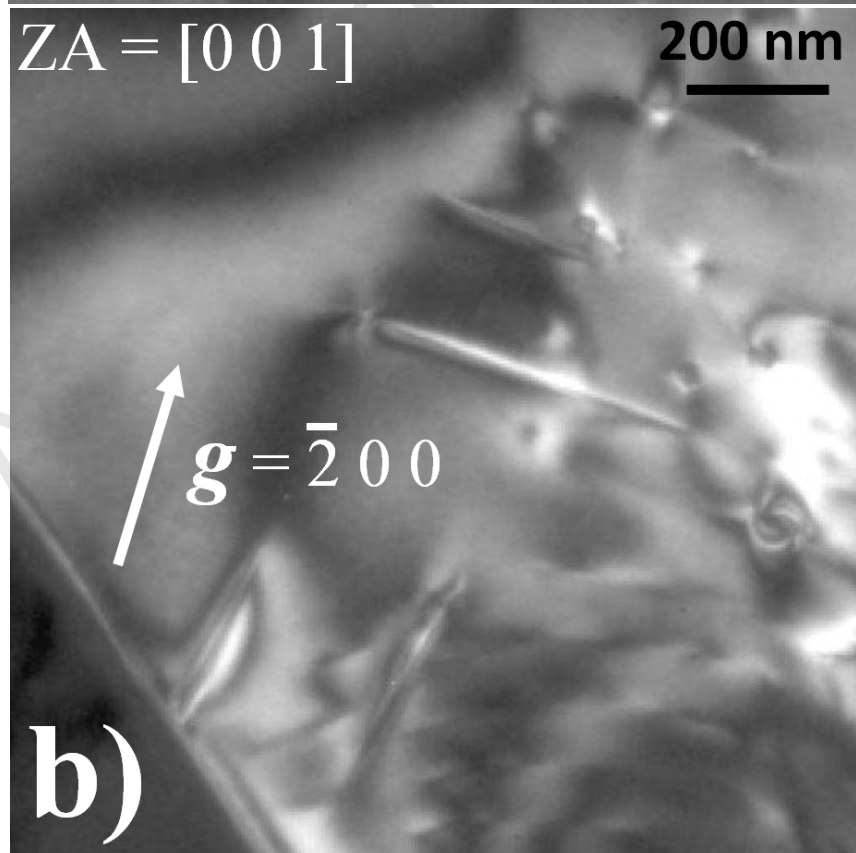
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Figure 5.



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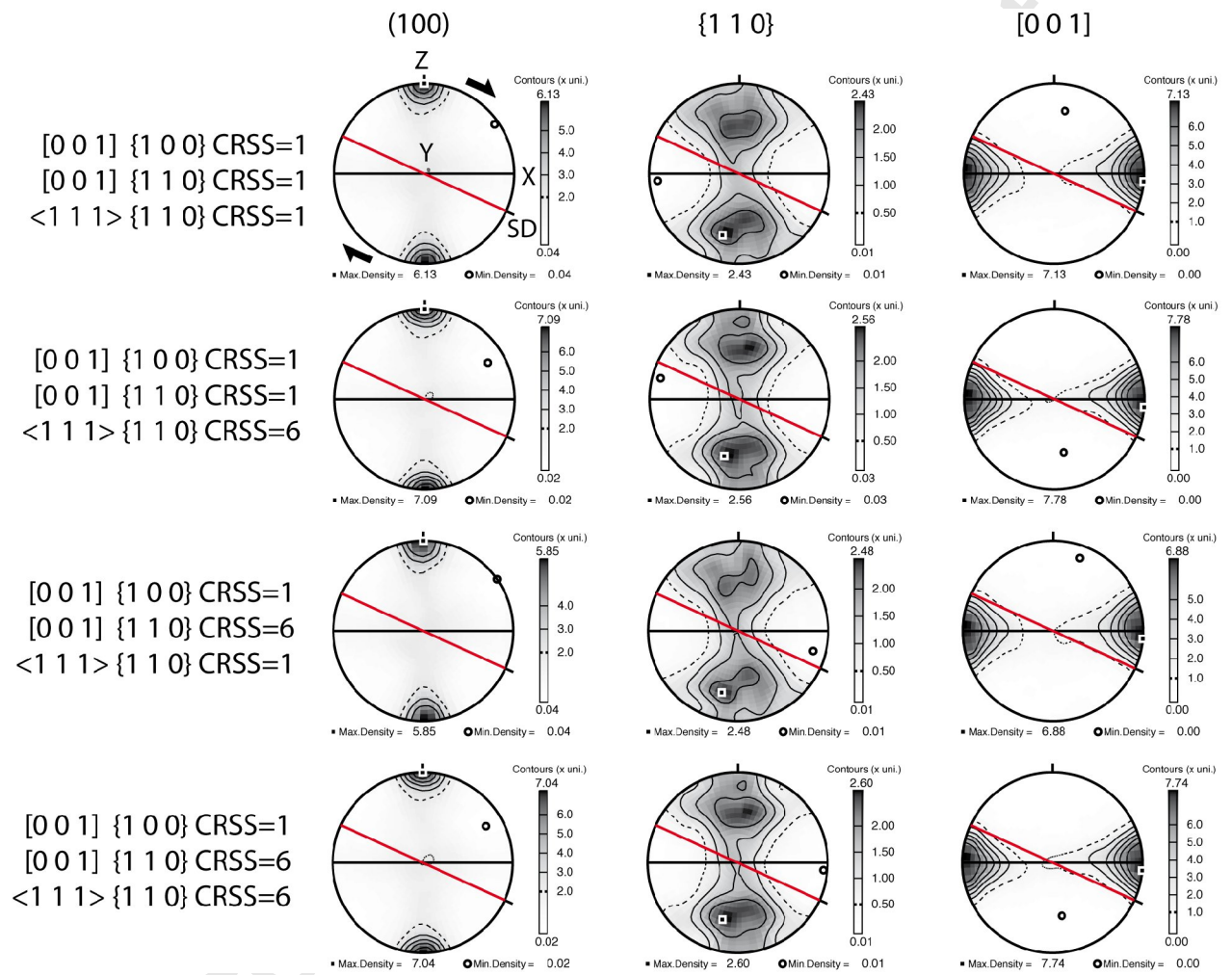
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Figure 6.

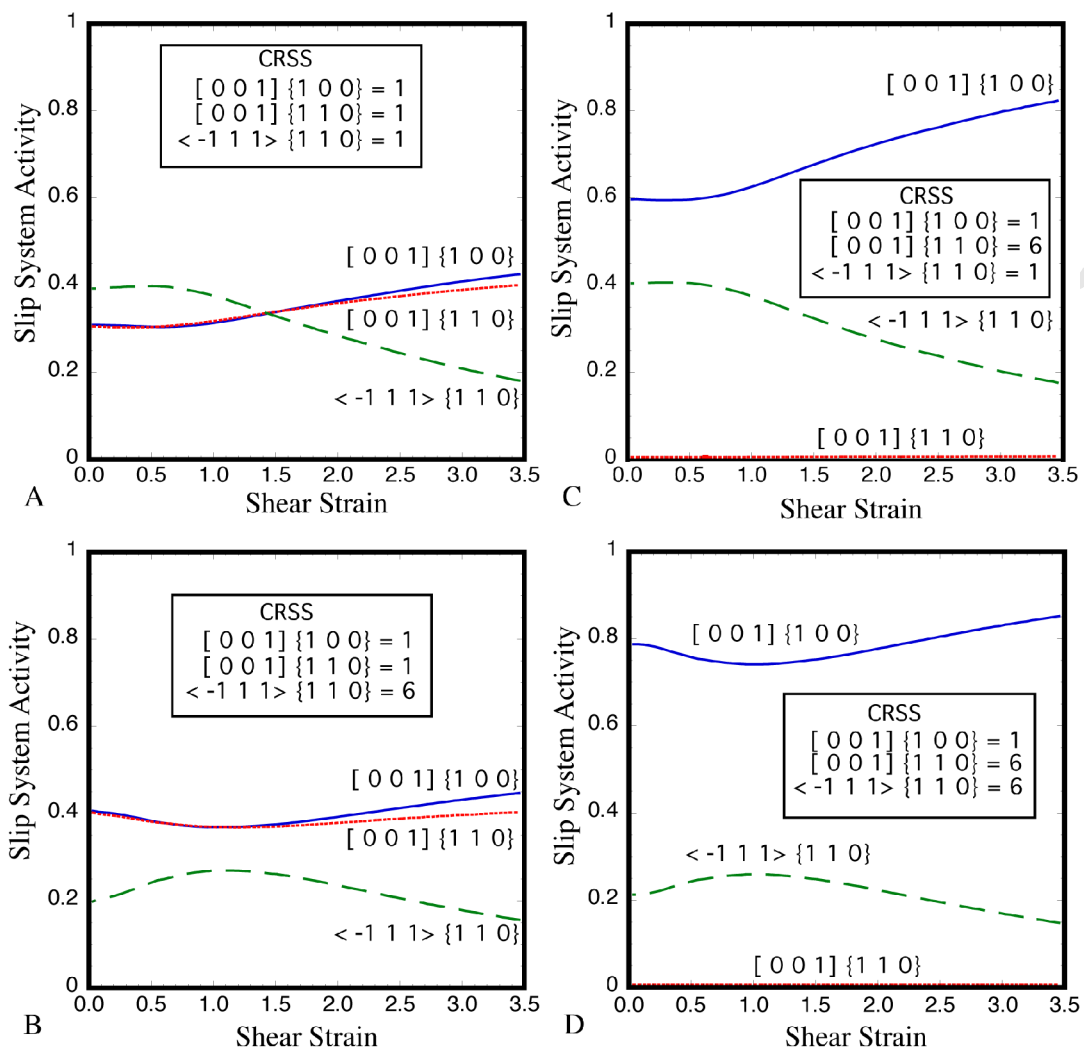


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Figure 7.

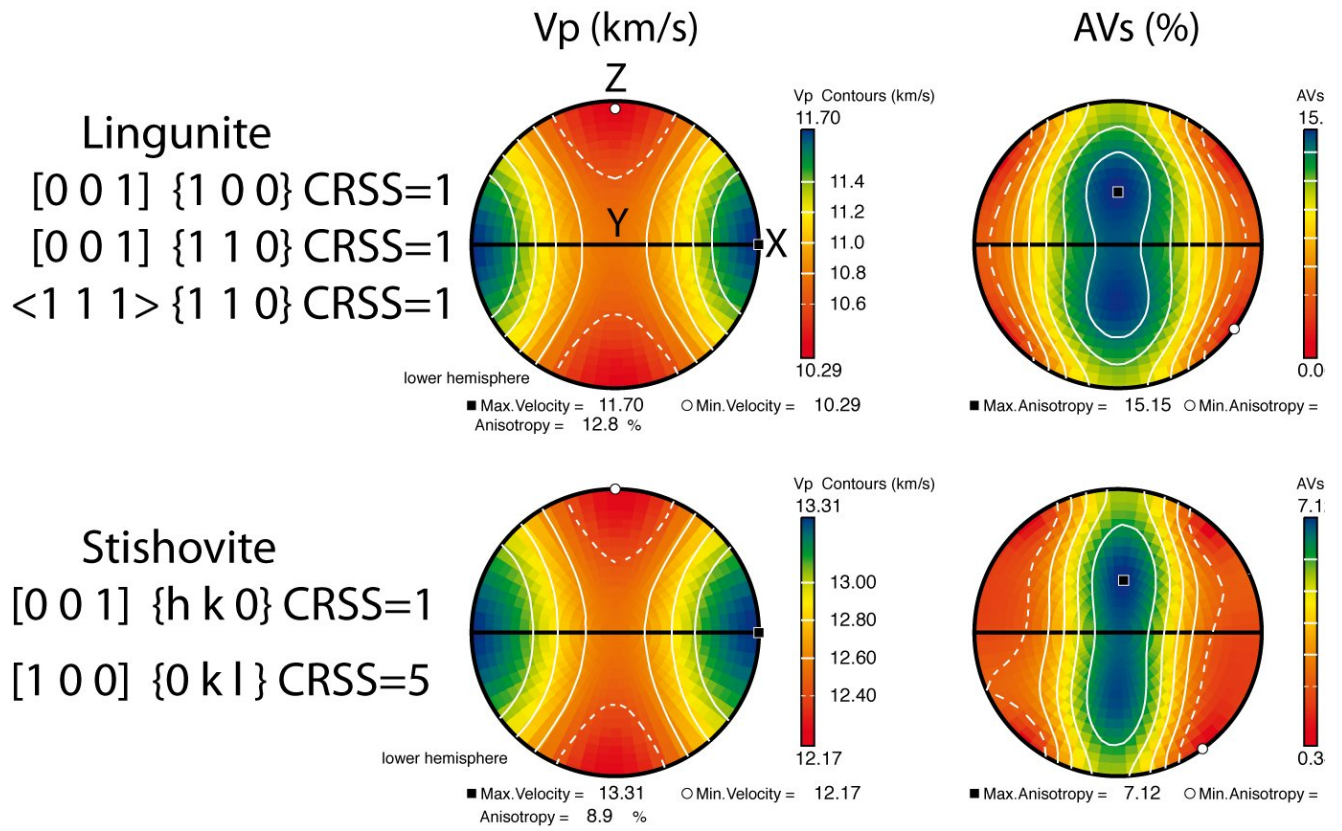


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Figure 8.

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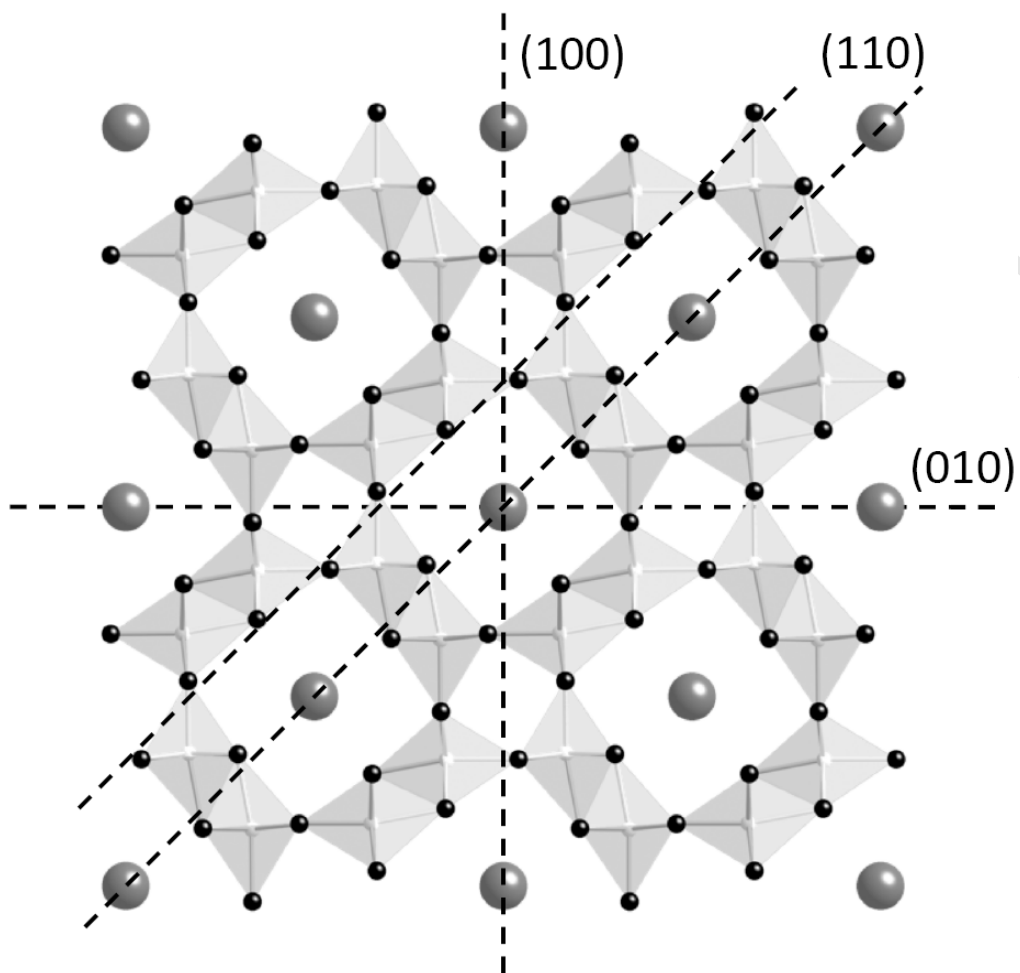


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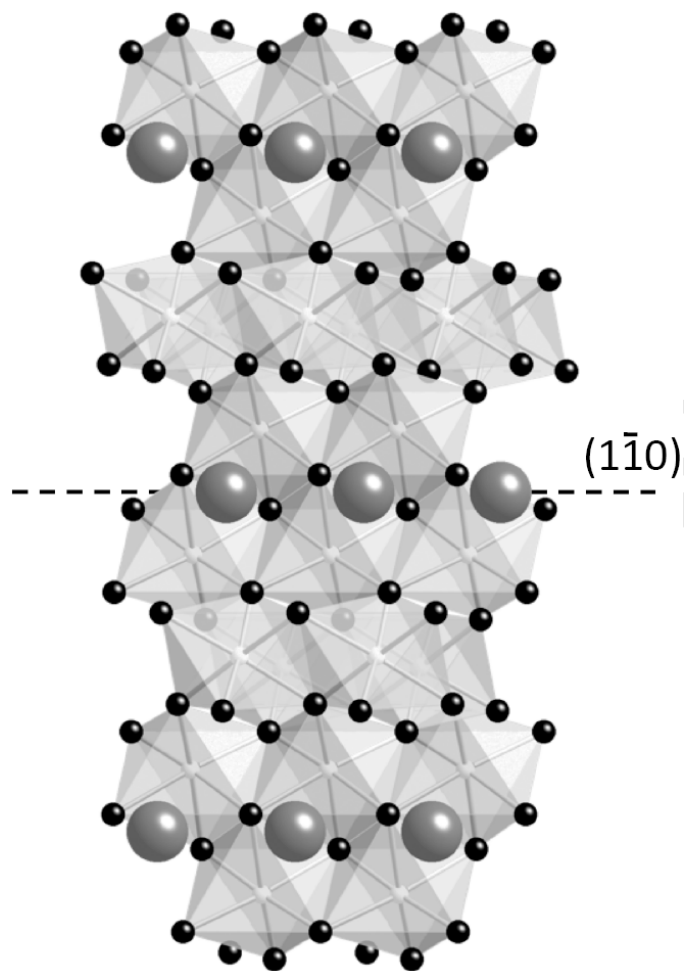
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Figure 9.



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Figure 10.

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611 **Table**

612 Table 1

g	g.b
$\bar{1}\bar{1}0$	0
$4\bar{5}1$	-1
$0\bar{3}1$	-1

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