Climb of jogs as a rate-limiting process of screw dislocations motion in olivine dislocation creep

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November 30, 2022

Abstract

Dislocation recovery experiments were conducted on pre-deformed olivine single crystals at temperatures of 1,450 to 1,760 K, room pressure, and oxygen partial pressures near the Ni-NiO buffer to determine the annihilation rates constants for [001] (010) edge dislocations. The obtained rate constants were comparable with those of previously determined [001] screw dislocations. The activation energies for the motion of both dislocations are identical. This suggests that the motion of screw dislocations in olivine is not controlled by cross-slip but by the same rate-limiting process of the motion of edge dislocation, i.e. climb, at low-stress and high-temperature conditions. The diffusivity derived from dislocation climb indicates that dislocation recovery is controlled by pipe diffusion. The conventional climb controlled model for olivine can be applied to the motions of not only edge but also screw dislocations. The softness of the asthenosphere cannot be explained by the cross-slip controlled olivine dislocation creep.

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11 Abstract

Dislocation recovery experiments were conducted on pre-deformed olivine single crystals at 12 temperatures of 1,450 to 1,760 K, room pressure, and oxygen partial pressures near the Ni-NiO buffer 13 to determine the annihilation rates constants for [001] (010) edge dislocations. The obtained rate 14 15 constants were comparable with those of previously determined [001] screw dislocations. The 16 activation energies for the motion of both dislocations are identical. This suggests that the motion of 17 screw dislocations in olivine is not controlled by cross-slip but by the same rate-limiting process of 18 the motion of edge dislocations, i.e. climb, at low-stress and high-temperature conditions. The 19 diffusivity derived from dislocation climb indicates that dislocation recovery is controlled by pipe 20 diffusion. The conventional climb controlled model for olivine can be applied to the motions of not 21 only edge but also screw dislocations. The softness of the asthenosphere cannot be explained by the 22 cross-slip controlled olivine dislocation creep.

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Keywords: dislocation recovery, dislocation creep, temperature dependence, climb controlled model,
 asthenosphere

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27 Introduction

Geophysical observations regarding geoid (e.g. Hager, 1991) and post-glacial rebound (e.g. Peltier, 1998) suggested that a soft asthenosphere underlies a rigid lithosphere. Geodynamic modellings (e.g. Becker, 2017; Craig and McKenzie, 1986) also suggested the same conclusion. The reason for the soft asthenosphere is under debate. Although the simplest explanation is weakening of materials due to the high temperature, results of deformation experiments on dry peridotite implied that the high temperatures are insufficient to explain the softness of asthenosphere (Hirth and 34 Kohlstedt, 2003). Although a popular explanation is hydrous weakening of olivine (e.g. Mackwell et 35 al., 1985; Hirth and Kohlstedt, 2003), it is doubted by recent Si self-diffusion experiments (Fei et al., 36 2016; Fei et al., 2013) based on the assumption that dislocation creep is controlled by diffusion. Another possible explanation was proposed by Poirier and Vergobbi (1978). They suggested that, if 37 38 cross-slip of dissociated screw dislocations controls olivine dislocation creep, the estimated uppermantle viscosity would be one order of magnitude lower than that predicted by the climb controlled 39 model in the stress range from 10 to 100 bar. This potentially explains the softness of the 40 41 asthenosphere. However, there is no experimental study to test this hypothesis.

Neither diffusion nor deformation experiments can identify the rate-limiting process of motions 42 of screw dislocations. Diffusion does not involve motions of dislocations. Although it is theoretically 43 44 possible to determine the rate-limiting process of dislocation motions by examining the stress 45 dependence of creep rates (e.g. Hirth and Kohlstedt, 2003), the stress ranges in deformation 46 experiments are too narrow. Conventionally used stress exponent of 3.5 for dislocation creep implies 47 a pipe diffusion controlled mechanism (Hirth and Kohlstedt, 2003, 2015). However, those experiments have a stress range only from 100 to 224 MPa. On the other hand, Kohlstedt and Goetze 48 49 (1974) found that stress exponent increases with increasing stress. Poirier (1985, P.139) found that 50 the stress exponent of olivine single crystal dislocation creep varies from 2.6 to 3.7 in different studies. 51 In this study, we conducted dislocation recovery experiments on [001](010) edge dislocations 52 and compared the results with those of [001](010) screw dislocations from Wang et al. (2016). During recovery, dislocations move on the slip plane (glide) and out of the slip plane (climb, cross-slip) 53 successively under the influence of internal stress. Therefore, the activation energy determined by 54 55 this method represents that of the rate-limiting process of dislocation motions. Although the model

from Poirier and Vergobbi (1978) was based on [100] screw dislocations, most of them have edge character at temperature less than 1350 °C (Bai and Kohlstedt, 1992; Wang et al., 2016). On the other hand, the similar density of edge and screw dislocations in [001](010) slip system (Wang et al., 2016) indicates equivalent importance of both types of dislocations in this slip system. Therefore, we focus on this slip system in this study (here after called *c*-dislocations).

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62 **Experimental Procedure**

The same Pakistan olivine and sample preparation procedure as those of Wang et al. (2016) were employed in this study. The composition of olivine was reported by Gose et al. (2010). The experimental setup is similar with that in Wang et al. (2016). The olivine single crystal was orientated by X-ray diffraction and electron backscattered diffraction (EBSD), and then placed in the cell assembly such that the [001] direction and (010) plan are parallel to the shear direction and plane, respectively.

69 Dislocations with the [001] Burgers vector on the (010) plane were produced by experimental deformation using a Kawai-type multi-anvil apparatus at University of Bayreuth. The sample 70 71 assembly was first pressurized to 3 GPa with a press load of 3.6 MN, and then heated to a temperature of 1,600 K and held for 15 min to sinter crushable alumina. After that, the assembly was further 72 73 compressed to a press load of 3.9 MN for 15 min to deform the sample. After the deformation, the 74 sample was quenched by switching off the heating power, and then decompressed to room pressure for more than 16 hours. Transmission electronic microscopy (TEM) by Wang et al. (2016) found 75 [001](010) slip system was successfully activated and dominant by this procedure. The ratio of screw 76 to edge dislocations was 3:2, as reported by Wang et al. (2016). 77

78 The deformed olivine crystals were cut into eight cubic pieces, and paired into four groups, in 79 which the two pieces in each group shared a common (100) plane. One piece from each pair was used to determine the initial dislocation density, while the other was used to determine dislocation density 80 81 after the annealing. The annealing experiments were conducted at ambient pressure and temperatures 82 of 1,460 to 1,760 K for 35 min to 24 hours using a gas mixing furnace. The oxygen partial pressure was controlled at 10⁻⁶-10⁻⁸ MPa, which is near the Ni-NiO buffer, using a CO-CO₂ gas mixture. Table 83 84 1 summarizes conditions of the annealing experiments. 85 Dislocations were observed using oxidation decoration technique (Kohlstedt et al., 1976, Karato 86 1987). The corresponding areas away from sub-grain boundaries on the common (100) plane in the 87 initial and annealed pieces from the same group were observed to determine the change in dislocation 88 densities before and after annealing. Since [001](010) edge dislocations elongate in [100] direction, 89 these dislocations show dots contrast on (100) plane in backscattered images after decoration. The 90 dots per unit area were counted as the dislocation density. The annihilation rate constants were calculated using the second-order dislocation recovery 91 kinetics (Karato and Ogawa, 1982; Kohlstedt et al., 1980; Wang et al., 2016) 92 $k = \frac{\frac{1}{\rho_f} - \frac{1}{\rho_i}}{t},$ 93 (2)

94 where ρ_f and ρ_i are the dislocation densities after and before annealing, respectively, and *t* is the 95 annealing time. Because of the thermally activated process, the dislocation annihilation rate constant 96 is assumed to follow the Arrhenius relationship:

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$$k = k_0 \exp\left(-\frac{E}{RT}\right)$$
(3)

98 where k_0 is a constant, *E* is the activation energy of dislocation annihilation, *T* is the temperature, 99 and *R* is the gas constant. 100

101 **Results**

102 Table 1 shows experimental results together with the annealing conditions. Dislocation density in the samples before deformation is less than 0.0004 μ m⁻², which is negligible in comparison with 103 104 dislocation density after deformation (Table 1). Figure 1 a and b shows back-scattered electron images 105 of decorated dislocations in the corresponding areas in the samples from the same pair before and 106 after annealing, respectively. The *c*-screw dislocations appear as lines and the *c*-edge dislocations as 107 dots on the (100) plane due to their geometries. Decrease in dislocation density was observed by 108 comparing the images before and after annealing. The water contents in the samples before and after 109 annealing were below the detection limit of infrared spectroscopy. The transmission electron 110 microscope images of the dislocation structures after deformation were given in Fig. 4 in Wang et al. 111 (2016).

112 Figure 1c plots the logarithmic rate constants of c-edge dislocations annihilation against the 113 reciprocal temperature. The results from the previous dislocation recovery experiments on *c*-screw 114 dislocations (Wang et al., 2016) and from other studies on dislocation recovery kinetics are also 115 plotted in this figure. The dislocation annihilation rate constants of *c*-edge and *c*-screw dislocations 116 are comparable, but those of the *c*-screw are about half orders of magnitude higher than those of the 117 c-edge. The temperature dependences for these two dislocations are identical. Their activation 118 energies are $E_{c-edge} = 400 \pm 20$ kJ/mol and $E_{c-screw} = 400 \pm 30$ kJ/mol for the *c*-edge and *c*-screw, 119 respectively.

120

121 **Discussion**

The identical activation energies of annihilation rate constants of the *c*-edge and *c*-screw dislocations indicate that the motions of both dislocations are controlled by the same mechanism. Although many transport properties of olivine exhibit activation energies between 300 to 500 kJ/mol (e.g. Dohmen et al., 2002, 529 ± 41 kJ/mol for silicon self diffusion, 338 ± 14 kJ/mol for oxygen self diffusion), they are distinct from those determined in this study (also see the slope in Fig.3 and references there). The high accuracy in activation energies obtained in previous and this study allows us to distinguish the rate-limiting mechanisms of different processes.

The motion of edge dislocations is controlled by climb at high temperatures and low stresses 129 130 (e.g. Hull and Bacon, 2001; Kohlstedt, 2006). However, motion of a pure screw dislocation does not 131 involve climb because screw segments have no specific slip plane (Hull and Bacon, 2001). Since jogs 132 in screw dislocations has edge character, we propose that the motion of screw dislocation is controlled 133 by climb of jogs (Fig. 2). A screw dislocation can form a jog by cross-slips to overcome obstacles 134 that it meets during glide (Fig.2A and 2B). The slip plane of the jog is defined by its dislocation line 135 (J) and the Burgers vector (b), indicated by the yellow plane. The parent screw dislocation glides in the y direction and therefore, the jog needs to climb in the y direction to move along with their parental 136 137 dislocation so that the screw dislocation can go through the obstacle (Fig. 2C). This climb of jogs should serve as the rate-limiting process of the screw dislocation motions. 138

It is noted that although the climb of edge dislocation and jog motion of screw dislocation are essentially the same, the density of climbing parts on edge dislocations and that of jogs on screw dislocations may be different, which causes difference in magnitude of rate constants. Thus, only the slope in the Arrhenius plot can be a fingerprint of the essential mechanism of rate-limiting processes in dislocation recovery experiments.

Since climb is controlled by diffusion, the diffusivities derived from annihilation rate constants, 144 D^R (based on Karato and Ogawan, 1989) were compared with those of silicon and oxygen diffusion 145 in olivine (Fig. 3). None of these data fit D^R well. Instead, D^R fall between silicon lattice and grain 146 147 boundary diffusivities. This indicates that the dislocation climb in olivine may be controlled by pipe 148 diffusion. Vacancies, dislocations and grain boundaries are 0-, 1-, 2-dimension defects, the structure 149 distortion near these defects should increase consequently and accordingly, the associated Si diffusivity should increase consequently. In addition, the activation energy of D^R obtained in this 150 151 study is between those of Si lattice (540 kJ/mol, Dohmen et al., 2002) and grain boundary diffusion (~200 kJ/mol, Fei et al., 2015). This is also consistent with the hypothesis that pipe diffusion controls 152 153 dislocation climb. Although there is no data for the pipe diffusion in olivine, the fact that diffusion 154 coefficient and activation energy of pipe diffusion are between those of lattice and grain boundary 155 diffusion are well established in oxides (Frost and Ashby, 1983, Table 12.1). The low activation 156 energy of oxygen lattice diffusion (~340 kJ/mol, Dohmen et al., 2002) rules out the possibility that 157 oxygen diffusion controls dislocation climb.

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159 Implications

It was proposed that the softness of asthenosphere can be explained by the cross-slip controlled dislocation creep of olivine (Poirier and Vergobbi, 1978). However, this hypothesis was never tested. The present study demonstrates that motion of [001] screw dislocations is controlled by climb of jogs rather than cross-slip, suggesting that cross-slip model is not applicable for such dislocations in olivine. Although the cross-slip model is based on [100] dislocations, study of [001](010) slip system is more relevant to the asthenosphere conditions. Dislocation structure analyses indicated that most

[100](010) dislocations have edge character (Bai and Kohlstedt, 1992, Wang et al., 2016), indicating 166 167 that olivine dislocation creep cannot be controlled by the motions of [100] screw dislocation. On the other hand, the similar density (Wang et al., 2016) of edge and screw dislocations in [001](010) slip 168 169 system indicates that both kinds of dislocations are important. Moreover, deformation experiments 170 (e.g. Raterron et al., 2007) suggested that this slip system dominated at high pressure. Therefore, we 171 conclude that cross-slip of screw dislocations cannot control the dislocation creep of olivine and accordingly, it cannot explain the softness of asthenosphere. The climb controlled model can be used 172 173 in olivine dislocation creep regardless of dislocation characters.

The viscosity of asthenosphere extrapolated from dry olivine creep data using climb model is 174 175 orders of magnitude higher than the estimated value from geophysical observation (Hirth and 176 Kohlstedt 2003). Hydrous weakening of olivine was proposed to explain this discrepancy (e.g. 177 Mackwell et al., 1985; Hirth and Kohlstedt, 2003) but it was disparaged by recent Si diffusion 178 experiments (Fei et al., 2016; Fei et al., 2013). However, this study indicates that pipe diffusion, rather 179 than lattice or grain boundary diffusion, may control the dislocation motions. This may explain the discrepant results between deformation and diffusion experiments. Further studies on the effect of 180 181 water on the dislocation recovery or pipe diffusion in olivine are needed to identify the effect of water 182 on the olivine rheology and to better explain the softness of the asthenosphere.

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187 Acknowledgements

We thank H. Fischer, R. Njul in BGI for the sample and assembly preparation. This research was
supported by DFG grants to TK (KA3434-3/1, KA3434-3/2, KA3434-7/1 and KA3434-8/1) and by
the annual budget of BGI. All data used in this paper are in Table 1 and plotted in Figure. 1c

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256 Figure and table captions

Figure 1. BEIs showing the dislocation density (a) before and (b) after annealing at 1760 K for 35 minutes. The images were taken on the (100) plane. Screw and edge dislocations are lines and dots, respectively, due to the geometries of their dislocation lines. The yellow scale bar represents 2 μ m. (c) Logarithmic dislocation annihilation rate constants of *c*-edge dislocations versus reciprocal temperature. Together plotted are the annihilation rate constants of *c*-screw dislocations from Wang et al., (2016). The activation energies for both dislocations are identical, i.e. 400 kJ/mol. Previous results on dislocation recovery are also plotted for comparison.

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266 Figure 2. A schematic diagram showing the jog-climb controlled motion of a screw dislocation. (a) The screw dislocation (blue line) is elongated in the x direction, which is parallel to its Burgers vector 267 **b**, and glides in the *y* direction. The blue dot represents the obstacle that the screw dislocation meets 268 269 during glide. (b) A jog (red segment) elongated in the z direction is produced on the screw dislocation in order to overcome the obstacle. This jog has an edge nature with the same Burgers vector **b** as the 270 271 parental screw dislocation. The yellow area indicates the glide plane of the jog, which is normal to the *y* direction. (c) The jog has to climb out of its glide plane in order to move along with its parental 272 273 screw dislocation.

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Figure 3. Logarithmic diffusivity derived from dislocation annihilation rate constants of *c*-edge and *c*-screw dislocations versus reciprocal temperature. Together plotted are Si and O lattice and grainboundary diffusivities.

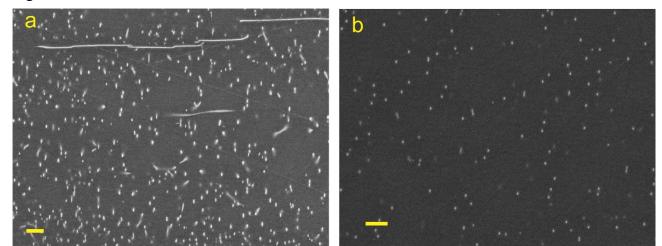
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- 280 Table 1. Summary of experiment conditions and results.
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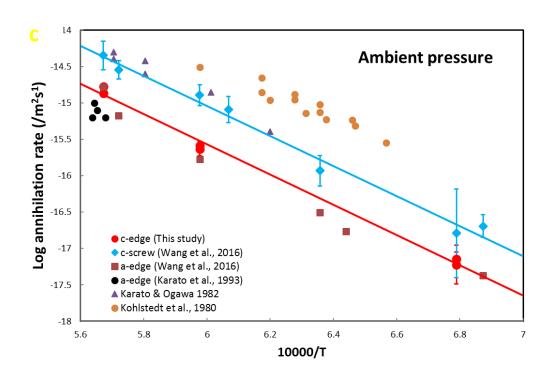
282 Table 1. Summary of experimental conditions and results*.

[001](010) edge dislocation								
Sample	Т	Annealing	$\log(f_{0_2}, 10^5)$	$\rho_i (\mu m^{-2})$	$\rho_f(\mu m^{-2})$	$\log(k, \mathrm{m}^2\mathrm{s}^{-1})$		
	(K)	time (h)	Pa)					
Z1643-1	1763	0.58	-4.9	1.60 ± 0.13	0.29 ± 0.01	-14.87 ± 0.03		
				0.97 ± 0.13	0.22 ± 0.01	-14.77 ± 0.03		
Z1643-2	1673	2.5	-5.7	1.49 ± 0.04	0.36 ± 0.06	-15.63 ± 0.09		
				1.13 ± 0.12	0.31 ± 0.03	-15.58 ± 0.05		
Z1643-3	1473	24	-7.7	1.33 ± 0.15	0.73 ± 0.05	-17.14±0.09		
				0.35 ± 0.03	0.29 ± 0.01	-17.22 ± 0.27		

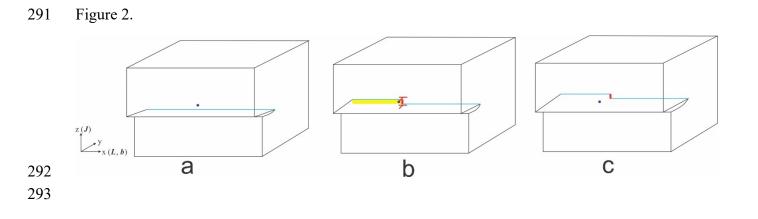
* different ρ_i and ρ_f in each sample correspond to different areas

Figure 1.





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294 Figure 3.

