**Elasticity of akimotoite under the mantle conditions:** **Implications for multiple discontinuities and seismic anisotropies at the depth of**

**~600-750 km in subduction zones**

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**Table S1**. Elastic moduli and their pressure derivatives of akimotoite at 0 GPa

**Table S2**. Elastic moduli and their temperature derivatives of akimotoite at 300K

**Table S3**. Wave velocities and their first and second derivatives

**Table S1**. Elastic moduli and their pressure derivatives of akimotoite at 0 GPa

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| T (K) | C11 | C12 | C13 | C33 | C44 | C14 | C25 | KS | G |
|  | M0 (GPa) | | | | | | | | |
| static | 461 | 156 | 92 | 373 | 112 | -28 | -16 | 212 | 132 |
| statica | 444 | 173 | 122 | 383 | 90 | -24 | -28 | 234 | 120 |
| staticb | 477 | 153 | 89 | 392 | 121 | -28 | -16 | 222 | 144 |
| 300 | 443 | 148 | 82 | 353 | 104 | -25 | -17 | 204 | 127 |
| 298\*c | 472 | 168 | 70 | 382 | 106 | -27 | -24 | 212 | 132 |
| 300\*d |  |  |  |  |  |  |  | 218.9(6) | 131.2(3) |
| 300e | 476 | 155 | 102 | 383 | 114 | -29 | -26 | 226 | 136 |
| 1000 | 420 | 143 | 74 | 329 | 92 | -17 | -18 | 191 | 118 |
| 1500 | 402 | 139 | 67 | 310 | 82 | -10 | -18 | 181 | 110 |
| 1500f | 380 | 159 | 89 | 319 | 79 | -27 | -18 | 192 | 94 |
| 2000 | 383 | 135 | 61 | 290 | 72 | -4 | -19 | 171 | 100 |
|  |  | | | | | | | | |
| static | 5.65 | 3.26 | 3.89 | 5.61 | 2.11 | -0.53 | 0.25 | 4.36 | 1.55 |
| statica | 6.64 | 3.76 | 4.97 | 6.17 | 2.48 | 0.30 | -0.48 | 5.20 | 1.66 |
| staticb | 6.0 | 3.5 | 3.9 | 5.7 | 2.2 | -0.4 | 0.3 | 4.5 | 1.6 |
| 300 | 5.76 | 3.21 | 3.87 | 5.78 | 2.19 | -0.58 | 0.24 | 4.39 | 1.64 |
| 300\*d |  |  |  |  |  |  |  | 4.62(3) | 1.64(1) |
| 300e | 4.65 | 3.51 | 3.82 | 3.34 | 1.78 | 0.30 | -0.36 | 3.85 | 1.04 |
| 1000 | 6.03 | 3.18 | 3.92 | 6.17 | 2.36 | -0.67 | 0.24 | 4.52 | 1.83 |
| 1500 | 6.25 | 3.14 | 3.93 | 6.50 | 2.51 | -0.75 | 0.23 | 4.61 | 2.00 |
| 2000 | 6.48 | 3.07 | 3.94 | 6.88 | 2.68 | -0.85 | 0.22 | 4.71 | 2.22 |
|  | ( GPa-1) | | | | | | | | |
| static | -17.30 | 0.26 | -4.36 | -25.27 | -10.52 | 3.74 | 0.40 | -9.07 | -10.63 |
| 300 | -18.06 | 0.71 | -4.17 | -26.56 | -11.12 | 4.15 | 0.47 | -9.24 | -11.33 |
| 1000 | -20.13 | 1.48 | -4.16 | -30.10 | -12.76 | 5.04 | 0.56 | -10.09 | -13.28 |
| 1500 | -21.89 | 2.34 | -3.98 | -33.26 | -14.23 | 5.89 | 0.66 | -10.72 | -15.20 |
| 2000 | -23.92 | 3.50 | -3.66 | -37.01 | -15.99 | 6.93 | 0.79 | -11.42 | -17.73 |

The data are fitted based on the equation: ; *M* represents the elastic moduli; *P* is pressure in GPa. The fitting range of pressure is 0-40 GPa.

a Matsui et al. (1987), semi-empirical calculations; b Da Silva et al. (1999), first-principles calculations; \*c Weidner and Ito (1985), Brillouin spectroscopy; \*d Zhou et al. (2014), ultrasonic interferometry techniques; e Zhang et al. (2005), classical molecular dynamic calculations; f Li et al. (2009), 1500 K, 0.9(2) GPa, first-principles molecular dynamic calculations. The experimental data are marked by \*, and the data without symbols are from this study.

**Table S2**. Elastic moduli and their temperature derivatives of akimotoite at 300 K

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| P  (GPa) | C11 | C12 | C13 | C33 | C44 | C14 | C25 | KS | G |
|  | M0 (GPa) | | | | | | | | |
| 0 | 443 | 148 | 82 | 353 | 104 | -25 | -17 | 204 | 127 |
| 0\*a | 472 | 168 | 70 | 382 | 106 | -27 | -24 | 212 | 132 |
| 0\*b |  |  |  |  |  |  |  | 218.9(6) | 131.2(3) |
| 0c | 476 | 155 | 102 | 383 | 114 | -29 | -26 | 226 | 136 |
| 10 | 500 | 181 | 121 | 410 | 126 | -30 | -15 | 248 | 143 |
| 20 | 552 | 213 | 158 | 459 | 144 | -35 | -12 | 289 | 156 |
| 30 | 600 | 246 | 195 | 504 | 160 | -39 | -9 | 328 | 167 |
|  | (MPa/K) | | | | | | | | |
| 0 | -32.34 | -7.97 | -11.55 | -32.14 | -16.39 | 11.34 | -1.19 | -17.91 | -12.42 |
| 0\*b |  |  |  |  |  |  |  | -19.9(9) | -15.8(4) |
| 0c | -41.6 | -10.0 | -13.2 | -37.3 | -19.7 | 0.00 | 2.5 | -21.6 | -17.9 |
| 10 | -28.90 | -8.14 | -10.84 | -27.32 | -14.26 | 10.33 | -1.25 | -16.21 | -10.30 |
| 20 | -26.23 | -8.02 | -10.15 | -23.83 | -12.73 | 9.62 | -1.27 | -14.83 | -8.83 |
| 30 | -24.05 | -7.76 | -9.48 | -21.14 | -11.57 | 9.10 | -1.27 | -13.66 | -7.74 |
|  | ( GPa/K2) | | | | | | | | |
| 0 | -2.01 | -0.004 | -0.69 | -3.12 | -1.49 | 0.68 | -0.01 | -1.26 | -1.94 |
| 0\*b |  |  |  |  |  |  |  | -2.9(8) | -6.7(4) |
| 10 | -1.58 | -0.44 | -0.92 | -2.18 | -1.04 | 0.37 | -0.06 | -1.18 | -1.14 |
| 20 | -1.32 | -0.68 | -1.04 | -1.64 | -0.79 | 0.19 | -0.09 | -1.14 | -0.75 |
| 30 | -1.16 | -0.82 | -1.11 | -1.31 | -0.64 | 0.08 | -0.11 | -1.11 | -0.53 |

The data are fitted based on the equation: ; *M* represents the elastic moduli; *T* is temperature in Kelvin. The fitting range of temperature is 270-2000 K.

\*a Weidner and Ito (1985); \*b Zhou et al. (2014); c Zhang et al. (2005). Their respective methods are shown in the caption of Table S1. The experimental data are marked by \*, and the data without symbols are from this study.

**Table S3**. Wave velocities and their first and second derivatives

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| P (GPa) | (km/s) | ( km/s/K) | ( km/s/K2) | (km/s) | ( km/s/K) | ( km/s/K2) |
| 0 | 9.955 | -0.327 | -5.993 | 5.806 | -0.204 | -5.438 |
| 0\*a | 10.11 |  |  | 5.90 |  |  |
| 0\*b | 10.211(8) | -0.352(12) | -12.2(11) | 5.862(6) | -0.253(9) | -13.9(8) |
| 10 | 10.542 | -0.252 | -3.215 | 6.022 | -0.154 | -2.538 |
| 20 | 11.010 | -0.202 | -2.015 | 6.168 | -0.122 | -1.358 |
| 30 | 11.399 | -0.170 | -1.376 | 6.271 | -0.100 | -0.758 |
| T (K) | (km/s) | ( km/s/GPa) | ( km/s/GPa2) | (km/s) | ( km/s/GPa) | ( km/s/GPa2) |
| static | 10.080 | 5.725 | -3.849 | 5.879 | 1.996 | -2.068 |
| 300 | 9.955 | 6.190 | -4.495 | 5.806 | 2.336 | -2.544 |
| 298\*a | 10.11 |  |  | 5.90 |  |  |
| 300\*b | 10.211(8) | 5.58(4) |  | 5.862(6) | 2.19(3) |  |
| 1000 | 9.696 | 6.915 | -5.362 | 5.634 | 2.877 | -3.241 |
| 1500 | 9.477 | 7.592 | -6.215 | 5.483 | 3.423 | -3.981 |
| 2000 | 9.224 | 8.448 | -7.352 | 5.298 | 4.164 | -5.038 |

The pressure derivatives are fitted based on the equation: , and the temperature derivatives are based on , where *V* represents *VP* or *VS*; P is pressure in GPa; T is temperature in Kelvin. The fitting range of temperature is 270-2000 K and the range of temperature is 0-40 GPa.

\*a Weidner and Ito (1985); \*b Zhou et al. (2014). Their respective methods are shown in the caption of Table S1. The experimental data are marked by \*, and the data without symbols are from this study.

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