Elasticity and rheology of iron above 220 GPa and the nature of the Earth's inner core

Russell J. Hemley ;, Baoheng L Y& An I K. Singh9
, eopIivsical Laboratory and Center for High Presure Research,
Carnegir Institution of Washington, 5251 Broad Branch Road, Y4S;
Washington DC 24015, USA
tConsortium far advanced Radiation Sources, University of Chicago, Chicago,
Illinois 64637, USA
lCenter for High Pressure Research, Mineral Physics Institute, State Vinuversuyat
stony Brook, Stan, Brook, New York 11794-2100, USA
,',i terials Science Division, National Aerospace Labora tories, Ba nga lore 560017,
1n&a

Recent numerical-modelling and seismological results have raised new questions about the dynamics`·' and magnetism of the Earth's core. Knowledge of the elasticity and texture of iron s'' at core pressures is crucial for understanding the seismological observations, such as the low attenuation of seismic waves, the low shear-wave velocity and the anisotropy of compressional-wave velocity -". The density and bulk modulus of hexagonal-close-packed iron have been previously measured to core pressures by static" and dynamic"·" methods. Here we study, using radial X-ray diffraction [15] and ultrasonic techniques', the shear modulus, single-crystal elasticity tensor, aggregate compressional- and shear-wave velocities, and orientation dependente of these velocities in iron. The inner core shear-wave velocity is lower than the aggregate shear-wave velocity of iron, suggesting the presence of low-velocity components or anelastic effects in the core. Observation of a strong lattice strain anisotropy in iron samples indicates a large (--24% compressional-wave anisotropy under the isostress assumption, and therefore a perfect alignment of crystals would not be needed to explain the seismic observations. Alternatively the strain anisotropy may indicate stress variation due to preferred slip systems.

Two radial X-ray diffraction (RXD) experiments (runs 1 and 2; see Fig. 1) were performed with diamond cells. Non-hydrostatic stress, a condition essential to the technique, was deliberately produced in the specimen by not adding a pressure medium. The stress state of the specimen *compressed between two anvils is a* superposition of the hydrostatic pressure

$$\sigma_P = (\sigma_3 + 2\sigma_1)/3 \quad (1)$$

and the differential stress components

$$t = \sigma_3 - \sigma_1 = 1.5(\sigma_3 - \sigma_P) \quad (2)$$

where σ_3 and σ_1 are axial and radial stresses, respectively[17]. A microfocus (4–10-μm diameter) polychromatic X-ray beam, which passed through the Be gasket in the radial direction, probed the lattice strain of the sample as a function of the angle (ψ) to the diamond-cell axis[15]. At 21 pressures between 16 and 211 GPa, energy dispersive X-ray diffraction (EDXD) patterns containing (*hkl* notation) 100, 002, 101, 102, 110, 103, 112, 201 diffraction lines of hexagonal close packed (h.c.p.) iron, 111, 200, 220, 311, 222, 400, 331, 420, 422, 511 of gold, or 110, 200, 211, 220, 310, 222, 321, 400 of tungsten, were collected at 10° steps of ψ from 0° to 90°. The *d*-spacing varies linearly with $\cos^2\psi$:

$$d(hkl) = d_P(hkl)[1 + (1 - 3\cos^2\psi)Q(hkl)] \quad (3)$$

where the intercept $d_P(hkl)$ denotes the *d*-spacing under σ_P, and the slope $Q(hkl)$ is the lattice strain under the uniaxial stress condition[18,19].

In run 1, a separate gold layer was used as a standard for determination of *t* and shear modulus *G* of h.c.p. Fe. The axial stress is continuous across the interface between the gold and iron layers ($\sigma_{3Au} = \sigma_{3Fe}$; subscripts denote the Au or Fe layer), that is

$$t_{Fe} = 1.5(\sigma_3 - \sigma_{PFe}) = 1.5(\sigma_{PAu} - \sigma_{PFe}) + t_{Au} \quad (4)$$

Now, *t* is related to *G* by

$$t = 6G\langle Q\rangle \quad (5)$$

where $\langle Q\rangle$ denotes the average value of measured *Q* for all (*hkl*) (ref. 15). The hydrostatic stress components, σ_{PAu} and σ_{PFe}, were determined from the observed $d_P(hkl)$ (equation (3)) and the equations of state of Au and Fe (refs 20, 21); G_{Au} was extrapolated from low-pressure data[22,23]. The aggregate compressional-wave speed (v_P) and shear-wave speed (v_S) of h.c.p. Fe are calculated from the bulk modulus K_{Fe} and G_{Fe}. In addition (run 3), the aggregate ultrasonic

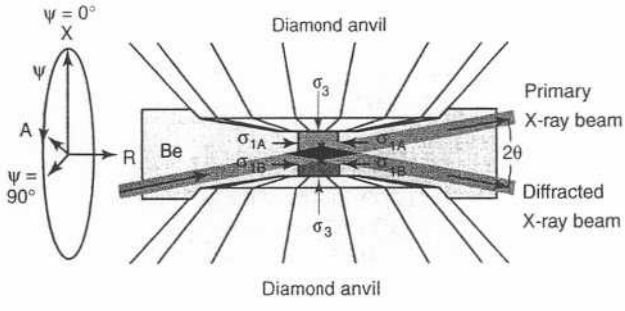
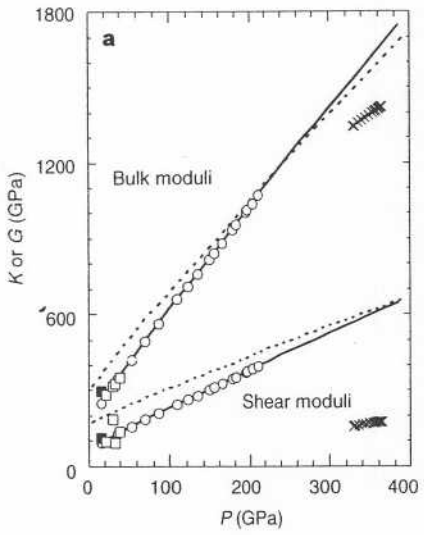


Figure 1 Lattice strains of diamond-cell samples under uniaxial stress (σ_1 and σ_3) are obtained with radial X-ray diffraction (RXD) through a beryllium gasket. The subscripts A and B denote the sample and stress standard. The vertical scale of the sample region is expanded. In run 1, the specimen, which consisted of a 15-μm (thickness) layer of an iron sample and a 3-μm layer of a gold standard, was compressed in a 40-μm (diameter) hole in a beryllium gasket between flat diamond anvils of 400-μm diameter. In run 2, the specimen consisted of a 5-μm iron and a 2-μm tungsten layer in a 15-μm hole in a Be gasket between bevelled diamond anvils (500-μm outer diameter, 90-μm inner diameter, 9.5° bevel angle). The diamond cell was mounted on a rotation stage with the diamond anvil axis (*A*) perpendicular to the rotation axis (*R*) which bisected the 2θ angle between incident and diffracted X-ray beams. The angle (ψ) between *A* and the diffraction vector (*X*) was varied as the diamond cell rotated around the *R* axis.

Table 1 Elasticity of h.c.p. Fe at 298 K and high pressures

P (GPa)	Density (g cm^{-3})	C_{11} (GPa)	C_{12} (GPa)	C_{33} (GPa)	C_{13} (GPa)	C_{44} (GPa)	K (GPa)	G (GPa)	v_P (km s^{-1})	v_S (km s^{-1})	Run no.
16.5	9.00*						297	108	6.95	3.47	3
39	9.67*	504	244	493	254	271	351*	134	6.84	3.76	1
39	10.09	747	301	802	297	215	455	224	7.86	4.72	†
211	12.61‡	1303	637	1302	637	960	1071‡	396	10.42	5.61	2
211	12.80	1697	809	1799	757	421	1085	445	10.54	5.90	†

Runs 1, 2 and 3 are results of this study. They are compared with values from first-principles calculations[6]. (The method and results of ref. 24 are similar to those of ref. 6.) Uncertainties for *K* and v_P, 10% (runs 1 and 2), 2% (run 3); for C_{ij}, *G* and v_S, 20% (runs 1 and 2), 2% (run 3).
* Ref. 21.
† Ref. 6.
‡ Ref. 12.



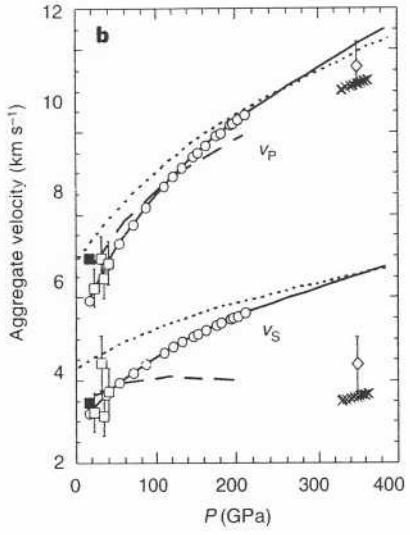


Figure 2 Comparison of our results with theoretical and shock-wave studies, and with seismic observations[25] in the inner core (crosses). Parameters compared are shear moduli and bulk moduli (**a**), and aggregate v_S and v_P (**b**) of h.c.p. Fe. Filled squares, ultrasonic measurements with multianvil apparatus in run 3; open squares, RXD measurements in run 1; solid curves, extrapolation of X-ray data in run 2 based on $K/G = 2.7$; short-dashed curves, first-principles calculations[6] for 298 K isotherm; long-dashed curves, shock-wave Hugoniot at high temperatures[13,14]. The solid curve was also used to calculate G and t for run 2 (open circles) for elasticity tensor estimations to 211 GPa. At 200 GPa, the differences between the Hugoniot values at 4407 K and the present 298 K values yield temperature derivatives; for example, $-dv_S/dT = 3.7 \times 10^{-4}$ km s^{-1} K^{-1} and $-dv_P/dT = 0.9 \times 10^{-4}$ km s^{-1} K^{-1}. In comparison with other estimations based on theory of thermal and elastic properties[30], this value of $-dv_S/dT$ is high, and $-dv_P/dT$ is low, possibly owing to the combined uncertainty in extrapolation of two data sets from entirely different studies (shock-wave and static compressions). If these derivatives are used for temperature correction of the solid curve to inner-core conditions, the resulting v_S and v_P of h.c.p. Fe at 6,000 K and 350 GPa (open diamonds in **b**) represent upper and lower bounds, respectively; that is, the differences between open diamonds and crosses is significant for v_S, but not for v_P.

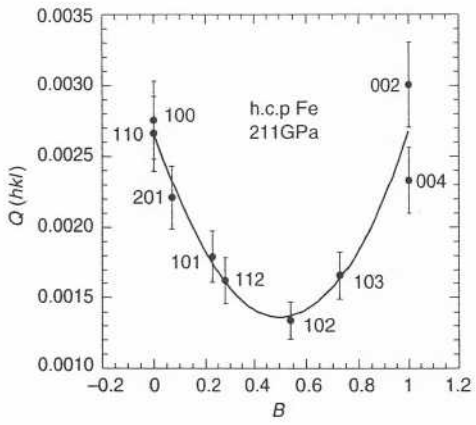


Figure 3 The measured $Q(hkl)$ of h.c.p. Fe at 211 GPa. This parameter follows a quadratic relation

$$Q(hkl) = m_0 + m_1 B + m_2 B^2 \quad (6)$$

where $B = 3a^2l^2/[4c^2(h^2 + hk + l^2) + 3a^2l^2]$. Under isostress assumption, the parameters m_0, m_1 and m_2 provide three independent linear equations for determination of elasticity tensors[15,27].

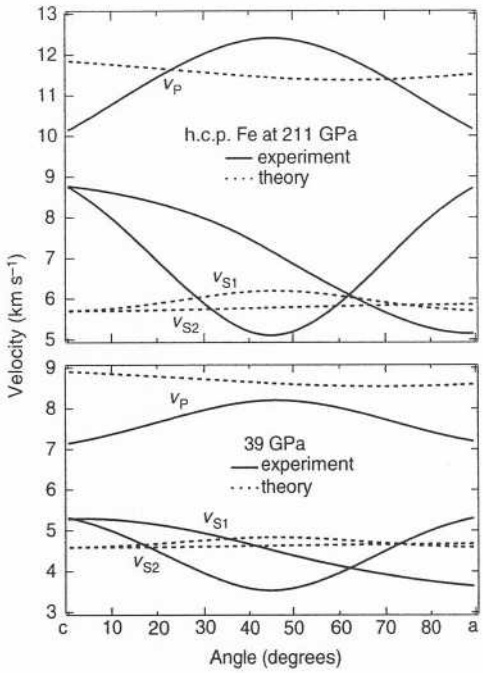


Figure 4 Comparison of seismic-wave velocities from this work with values calculated from theory. The velocities (v_P, v_{S1} and v_{S2}) of single-crystal h.c.p. Fe depend on the wave propagation direction relative to the c axis of the crystal. Solid curves, this study with isostress assumption; dashed curves, first-principles theory[6].

v_P and v_S of h.c.p. Fe are measured directly at 16.5 GPa in a multianvil press[16]. All experiments were performed at 298 K.

The results from RXD (zero-frequency) and multianvil (ultrasonic-frequency) measurements are in good agreement, bracketing a wide frequency range including seismic waves. The observed K/G ratio of h.c.p. Fe is 2.7(±0.7) from the RXD at 20–39 GPa, and is 2.68(±0.1) from the ultrasonic measurement at 16.5 GPa. We extrapolate G_{Fe}, t_{Fe}, v_P and v_S to higher pressures based on a constant K/G of 2.7, and compare the results with theoretical, shock-wave[13,14] and seismic values (Fig. 2). The K_{Fe}, G_{Fe}, v_P and v_S predicted by first-principles theory[6,24] are higher than the present values at low pressures, but the difference diminishes at higher pressures. Temperature derivatives of v_P and v_S are estimated from the differences between the Hugoniot data at high temperatures and the present static data at 298 K, and are used for estimation of v_P and v_S of h.c.p. Fe under the inner-core conditions[25] (Fig. 2b). The seismic v_S of the inner core is lower than the

co ponding h.c.p. Fe value_ If the softening of v_S represents possible :~)m-I)uraltd prernelting effects" or partial melting, the observed ,hear values would tightly constrain the inner-core temperature near melting, The near-melting softening would also attenuate seismic

Alternatively, the observations ma}} indicate the presence of a dditional low-v_S phases in the inner core.

The RXD measurements also provide single-crystal elasticity information Figure 3 shows that the Q(hk!) reaches a maximum at a (100, 110) and c (002) axes that is more than double the nlirti mum of the Q(hkl) at the diagonals (112, 102, 103). This trend persists over the entire pressure range studied. The strong *(hkl)* de pendence of lattice strain reflects a strong elasticity anisotropy or *an (hki)* dependence of stress"", which has little effect on the a forementioned estimates of averaged aggregate proprieties ["", *but* which gives information on single-crystal properties. Elasticity tensors and the orientation dependence of v_{p}, v_{s1} and v_{s2} (subscripts] and 2 denote two polarization directions) are calculated from parameters in equation (6) (see Fig. 3 legend) at the isostress limit"". Examples for h.c.p. Fe at 39 and 211 GPa are shown in Table I and Figs 2 and 4, and compared with values from first-principles theoretical predictions'. At 211 GPa (Fig. 3b), theories predicted a small vp anisotropy (4% faster in the c than in the a direction) which requires a perfect alignment ofh.c.p. Fe crystals (or a giant single crystal"") to account for the 4% inner-core v, anisotropy. The present results obtained under the isostress assumption show a large v_p anisotropy (24% faster at 45' from c than along either the a or the c axis), which relieves the `perfect alignment' textural constraint- Partial alignment of h.c.p. Fe crystals would be sufficient for the magnitude of inner-core anisotropy.

The isostress assumption for interpreting the data observed with our method has been confirmed experimentally for cubic phases of FeO and Fe (refs 15, 27). Its validity remains to be tested for hexagonal crystals. A strong (hkl) dependence oft (that is, non-isostress) in the polycrystalline specimen may partially or fully account for the observed lattice strain anisotropy. Consequently the elasticity tensor can no longer be uniquely determined, but is only partially constrained by the lattice Strain anisotropy in equation (6) with trade-offs among the values of the C_{ij} and textural parameters. For example, development of the basal-plane slip texture common in h.c.p. metals" could conceivably lower the t of grains with their c axis at 45° orientation. In such a case, the present observations at ultrahigh pressures, combined with elastic anisotropy information from theoretical estimates or single-crystal ultrasonic measurements at lower pressures, would yield theological information on single-crystal strength anisotropy and polycrystalline flow textures. Such information would affect our estimates of both elastic and anelastic anisotropies in the core[79].

Much information on bulk properties at high temperatures and pressures, and single-crystal elasticity and strength anisotropy, may be obtained by integrating techniques complementary to the three-dimensional RXD measurements reported here. These include ultrasonic studies, which provide accurate and direct determination of velocities below 20 GPa, hydrostatic X-ray diffraction, which provides Lattice parameters and bulk moduli to lnultimegabar pressures, shock-wave experiments, which determine bulk elasticity along the high pressure-temperature Hugoniot, and *ab* initio calculations, which provide independent determinations of elasticity. The present integrated study reveals that the elasticity of the Earth's inner core may represent the low shear modulus of h.c.p. Fe dose to melting, or the existence of additional components with low shear-wave velocities but similar density to Fe. As well as perfectly aligned h.c.p. Fe, more complicated textures should be considered,]ncluding partial alignment of these phases. D

"an'ed'4 March; accepted 17 September 1998.

Song, !(. & Richards. P. C,- Seismological evidence for differential rotation of the Earth's inner core. larnre 382,'21-224 f 19961.

Su, W.. Dxiewnn*i. A. N1. & lea nlon, R- Planet within a planet: rotation of the inner core of Earth. .tci.'s,c 274, 11133-133: ~ I996 l.

3. C,iat?n,aler. (7. A. & Robert'. P. II Rural ion and magnetism n1 Earth's inaer:on '. Srr. ·n :e 274, 188,- 139 r ! 1996:.
4. Kttang, 3K'-& Blo%harn. I. An earth-like numerical ds·namo maid. larure 389, 171 -374, 199'1-
5. ftphcoot..i. & 01,0,,. 1'. Is the in net core of the Farrh pure iroll !,valore 325, 332-3351 9871.
6. Stiarude. L. & Co hen, 19 1;- Hrgh-pressure elasticity of iron and anisorropv of FA rih's inner core.]..rear 267, 19---19-3 119931.
7. | ki:eonski, A 11 & Hillier.. F. Solidity nFthe inner core of the Earth inlcrred iron, normal mode nh,rnalien,. NA rure 234, 403-466 f 19711.
R. NJ asters. ` & f:ill,eri, I' Srrurlure of the nine. core inferred from obsrrs ·aiin rrs ii f its sphcrnidal sheaf m'Ill:,, · Gooplrr;. Res. tee'-8, 569-51-1119811.
9. Shearer · P. NJ.. Tov. K. 11. & ilreurt. I- A. Axi-symmetric Earth models and inner-core amsnlrnl,v. Varrrrc 333, '23- 232 1196111.
10. C reage r, K. C. An i;nt ro pi o trite inner core fro at d ifiereni is I t ravel times of i hr ph ase, PK P and PK 3 K P. Valore356, 3119-31411°921.
11. Tromp. I. So ppnn 501' anuni *ropy* of the Earth's inner COW rim free oirrliati.ms- 14u„r.366, 6:8-681 f1993i-
12. San_}i- K., Wu. Y.. (:hen. L. C., Shu, I- F. & !ephcoat. A. F Static compression of icon to 300 GPa and *Fe,* ' Alloy I o 260 < ;!?a; I mpl, a iocn for cn n, po si uu n a I the core. 1.. Geeplrys. Res. 95. Z I - 3 1 -2 1' 13 ! 199111.
13. Bmw-n.1. M. & 1taQuren. F. (.i. Phase-iransitinns, Gruneisen-parameter, and elastic.ir fir shocked iron hetweo,, ,, Gr'a and 400t,Pa0 I. Geaphys. Res. 91, ,435-'494 119a61-
14. Dulfv, F. S. C Ahrens. T 1. in High *Pressure Researrh: Ap plrc*.inn to E,rrflr and Ptniurar` Sciences (eds Siren. Y. & I,ianghnaai, 11. 11.1 35.1-361 f lerra Scientific Publishing, Tokyo, 19921.
15. Siugh, A. K.. Mao, H- K., Shu. 1. & Hemlcy, R. I. Estimation of singly-cr}-stal elastic moduli from pnls·ct%stalliitc x-r,,y dilir.rctiun at high pressure: Applications to Feo and iron. Phys. Rev. Let'. 80, 213: -'1160 11 9981-
16. Li. B.. Jackson, I.. 6-pa rik.1` & Lieberina an, R. C- Eli sticwasevelocit, measurement in multi-anvil apparatus to 1 *0* GPa using ultrasonic intcrfcmmetn-. *Plays. Earth* Planet. *Inrer.* 98, 79-91 119961.
17. F{elnrey, R. I. of af. N-rat imaging of stress and strain of diamond, iron, and lungeen 41 megabar pressures. 1,acirce 276, 1242-1245 119971.
18. Sigh. A. K. & 8:dasingh, C- The lattice strains in a specimen 1hexagnn ·,l svsleml compressed nonhydrostatically in an oppo,ed anvil high pressure setup-1. *Apps.* Phys. 75. 4936-4962119941.
19. tlehida. T., Fun amori, N. & 1'agi. T- Lattice strains in crystals under uniaxial stress field. *T Appr.* Phys. 80.739-746119961
20. Andrrson.0-L.. Isaak,1). G. & Yamamoto, 5. Anharmonicitv and *the* cgrration of stare for gold. `-Appl-Phl·s· 65, 1534-1513119891-
21. lepl,cna, A- I'.- e1 an. 1{. K. & Boll, P. Al. The static compression of iron ro 78 (iFs with rare gas solids as pressure-transmitting m dia- I- (iroph,t. Res- 11 91. 4677 .4684 :1986) -
22. Simmons, C. & Wang, H. Single Crystal Elastic Con<rrams and Calcnlaied Aggregate Hnperries (NUT Press, Cambridge, MA. 1971).
23. Guinan, NI. W. & 516 D", D. I- Pressure and temperature derivatives of the isotropic polyctyttallinc shear modulus for 65 elements-1. *Phys-Chem-* Solid< 35, 1501-1512 119741.
24. Suderliad, P., Moriarry, I-A. & Wills, I-11-first -prlncipies theorv of iron up to earth -corepressurcs Structural, vibrationa1. and elastic properties. Phys. Rev. 8 33, 14063 -14072 119961-
25. nzicwvnski. A. a.- Anderson, D- L- Preliminary reference earth model- Phys. Earth Planet. lure,- 25, 297-336119811-
'-6. Tal Ion, I. The volume dependence of elastic moduli and the Born -Durand melting hi ·pin hesis- Phil-Alas. 39. 151-161 1191-91.
27. Singh. A- K., Balasingh, C., Mac, H- K., Hemley, R. I- & 911 U.1. Analysis of lattice strains T110,urrd under no I,-hydrostat,c pressure. `. 4ppi. Phys. 83, 7567-7575 119981.
28. Weak, H. R., Takeshita, T. & leanloz, R. Development of tcxrure and elastic anisotropy during deformation of]icp metals. *Ceephys- Res-* Leer- 15. 76-l9 119881.
29. Romanowtca, B., Li, X. D. & Do rck, I. Anisutrops· in the inner core: on uld it he due to low-order copse lion? Science 274, 963. 966 11996).
30. 51 cry, F l7-Theory o1 thermal and elastic properties of the lower mantle and core. 1'3ys Earth Planet. Inter 89, 219-245 (1995).

Acknowledgements. We thank 1. Hu for technical help, L. Stixrude and R. E-Cohen for sharing theoretical data and discussions, T. Duff,- for comments, and NSLS and APS for synchrotron beam rime; the s,mchrnlron f cill(tes are supported by the DoE. This work was supported by the NSF.

Correspondence and requests for materials should be addressed to tl.M. (c- mail: h1AO@gl.ciw.edu) ·

Human longevity at the cost of reproductive success

Rudi G. J. Westendorp*† & Thomas B. L. Kirkwood†

** Section of Gerontology and Geriatrics, Department of General Internal Medicine, and Clinical Epidemiology, Leiden University Medical Centre CO-P, PO Box 9600, 2300 RC Leiden, The Netherlands*
† Biological Gerontology Group, Department of Geriatric Medicine and The School of Biological Sciences, University of Manchester, 3.239 Stopford Building, Oxford Road, Manchester M13 9PT, UK

The disposable soma theory on the evolution of ageing states that longevity requires investments in somatic maintenance that reduce the resources available for reproduction[1,2]. Experiments in *Drosophila melanogaster* indicate that trade-offs of this kind exist in non-human species[3–7]. We have determined the interrelationship between longevity and reproductive success in *Homo*