Supporting Online Material for

Dissociation of MgSiO$_3$ in the Cores of Gas Giants and Terrestrial Exoplanets

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Published 17 February 2006, Science 311, 983 (2006)
DOI: 10.1126/science.1120865

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References and Notes
I. Methods

Calculations were performed using the Mermin functional [S1,S2], and the local density approximation (LDA) [S3,S4]. Structural, vibrational, and thermodynamic properties were computed for electronic temperature, $T_{el} = 0$ K, 10,000 K and 20,000 K for comparison. The valence electronic configurations used for the generation of Vanderbilt ultrasoft pseudopotentials [S5] are: $2s^2 \ 2p^6 \ 3s^2 \ 3p^0 \ 3d^0$, $2s^2 \ 2p^6 \ 3s^1 \ 3p^0 \ 3d^0$, and $2s^2 \ 2p^4 \ 3d^0$, for Mg, Si, and O, respectively. Their cutoff radii are the same for all quantum numbers $l$ in each atom. They are 1.4 a.u., 1.2 a.u., and 1.0 a.u respectively. Transferability for these pseudopotentials, as quantified by logarithmic derivatives, are shown in Fig. S1. The plane-wave cutoff energy was 400 Ry. The unit cells of post-perovskite MgSiO$_3$, NaCl-type MgO, CsCl-type MgO, pyrite-type SiO$_2$, and cotunnite-type SiO$_2$ consist of two, one, one, four, and four formula units respectively. The numbers of $k$ points in the irreducible wedge of the Brillouin zone are 12, 10, 20, 4, and 6 respectively. We used variable-cell-shape molecular dynamics [S6] for structural
searches and optimization under arbitrary pressures. Dynamical matrices were computed at 6, 10, and 8 wave vectors $q$ for CaIrO$_3$-type MgSiO$_3$, CsCl-type MgO, and cotunnite-type SiO$_2$ respectively, using density-functional perturbation theory [S7]. Force constants are extracted to build dynamical matrices at arbitrary phonon $q$-vectors.

Structural stabilities in the relevant pressure range of each phase are investigated by inspecting phonon dispersions shown in Fig. S2A-C. Free energies were computed using the quasi-harmonic approximation [8] in conjunction with computed vibrational density of states. Calculations were carried out using the QUANTUM ESPRESSO package [S9]. Table S1 compares the calculated structural parameters with experimental values [S10,S11] and other calculations [S12] confirms the method’s computational capability. Table S2 reports numerical values of aggregate densities at various $PT$s for all phases. Compression curves are displayed in Fig. S3.

### II. ABX$_3$ Structures

Among the ABX$_3$ structures listed in Wyckoff [S13] and Hyde and Anderson [S14], the following metastable phases of MgSiO$_3$ have the lowest enthalpies at 12
Mbar: LiSbO$_3$-type, BaNiO$_3$-type, and hexagonal BaTiO$_3$-type (see Fig. S4 and Refs. S13 and S14 for more details). The LiSbO$_3$-type phase consists of SiO$_6$ octahedra interconnected in a $\alpha$-PbO$_2$-like network. This is a likely higher $P$ connectivity. In the BaNiO$_3$-type phase, SiO$_6$ octahedra share their faces and form separate columns. SiO$_6$ and MgO units are more segregated than in the CaIrO$_3$-type structure and could be a viable pre-dissociation phase. In the hexagonal BaTiO$_3$ structures, SiO$_6$ octahedra share their faces and apices. In these latter two structures silica octahedra have a higher degree of connectivity than the CaIrO$_3$ structure in which SiO$_6$ octahedra share edges and apices. The last $P6_3/mmc$ structure, to our knowledge, has not been observed experimentally so far. Its space group is a supergroup of the CaIrO$_3$ structure’s group. It was found by compressing uniformly the CaIrO$_3$ structure. Silicon is 8-fold coordinated and the silica polyhedra share edges and apices. The SiO$_8$ network is related to Ni$_2$In-type structure. These phases are dynamically stable. Their enthalpies relative to the CaIrO$_3$ phase’s at 12 Mbar are: 0.55, 0.89, 0.91, and 0.26 Ry/f.u., respectively.

III. Transport Properties
Our approach is to treat cotunnite-type SiO$_2$ as a semiconductor with thermally excited carriers which are scattered by intrinsic carrier-phonon and carrier-carrier processes and by extrinsic impurity scattering. The topic of transport in semiconductors is treated in many texts of which those by Ziman [S15], Blatt [S16], Ridley [S17], and Ferry [S18] are particularly useful. After the equations are described, in subsection III B5, page references to these books are given.

A. Carrier density

For predicting transport properties, it is desirable to use an approximate formula to describe the carrier density shown in Fig. 4. The standard semiconductor formula uses a parabolic band approximation, which we adopt for the conduction band (c) only. The density of states $N_c(\varepsilon)$ of this model is

$$N_c(\varepsilon) = \frac{2\pi}{E_c} \sqrt{\frac{\varepsilon}{E_c}}$$

where $E_c = \hbar^2 k_c^2 / 2m_c$ and $k_c = 2\pi / \Omega_c^{1/3}$. Using the cell volume of cotunnite-type SiO$_2$ at 10 Mbar, $\Omega_c = 276 a^3$, and the conduction band effective mass $m_c = 0.4m$, we get $E_c = 31.7$ eV. The parabolic approximation fails at relatively low $T$ for holes, since the valence bands are quite flat. Instead we use an alternate model, namely that holes
are localized with a maximum density of one hole per oxygen, with energy corresponding to the top of the valence (\(v\)) band. The density of states per unit cell is then

\[ N_v(\varepsilon) = 8\delta(\varepsilon - E_v). \]  \hspace{1cm} (2)

This model is motivated by the known tendency of electronic excitations to localize in low pressure SiO\(_2\) [S19]. The electron density is then found by standard statistical mechanics to be

\[ n(T) = 4\left(\frac{\Omega_c}{\lambda_{th}^3}\right)^{1/2} e^{-E_g/2k_BT} \approx \left(1.55 \times 10^{22} \text{cm}^{-3}\right)\left(\frac{T}{10^4 \text{K}}\right)^{3/4} e^{-E_g/2k_BT}. \]  \hspace{1cm} (3)

where the thermal de Broglie wavelength is \(\lambda_{th} = \sqrt{2\pi\hbar^2 / m_e k_BT}\), and the cell volume \(\Omega_c\) and effective mass \(m_e\) are chosen as 276 \(a_B^3\) and 0.4\(m\), values appropriate to cotunnite-type SiO\(_2\) at 10 Mbar, and where \(a_B\) and \(m\) are Bohr radius and electron mass.

The band gap from DFT is 5 eV. But in reality, we expect two compensating corrections, one that increases the gap to correct for DFT underestimations, and one that decreases the gap because of thermal fluctuations, mainly phonon renormalizations [S20]. Using \(E_g = 5\) eV at \(T = 10^4\) K, we find that nearly 0.9\% of SiO\(_2\) units have an excited electron and hole. This is a high carrier density, typical of semi-metals or very heavily doped
semiconductors, which have electrical conductivities typically one order of magnitude less than metallic values like $\sigma = 10^6 \Omega^{-1} \text{m}^{-1}$. The approximate formula in Eq. (3) agrees within 20% with the conventional calculations of Fig. 4B for $T \approx 10^4$ K.

**B. Electron scattering and electrical resistivity**

Electrical resistivity $\rho$ or conductivity $\sigma$ is conveniently factored into the $T$-dependent carrier density $n(T)$ and the more weakly $T$-dependent mobility $\mu(T)$ which depends on the scattering rate $1/\tau$.

$$1/\rho(T) = \sigma(T) = n(T) e \mu(T) \quad \text{and} \quad \mu = e \langle \tau(T) \rangle / m_e \quad (4)$$

What is actually calculated is the energy-dependent scattering rate $1/\tau(\varepsilon)$ which then has to be appropriately averaged over occupied states (whose number is proportional to $\sqrt{\varepsilon} \exp(-\varepsilon / k_b T)$) and weighted by the square of the velocity (which brings in another factor of $\varepsilon$). The averaging formula is

$$\langle \tau(T) \rangle = \frac{\int_0^\infty d\varepsilon \varepsilon^{3/2} \tau(\varepsilon) e^{-\varepsilon / k_b T}}{\int_0^\infty d\varepsilon \varepsilon^{3/2} e^{-\varepsilon / k_b T}}. \quad (5)$$

The generic form for electron-phonon scattering is

$$1/\tau_{\text{ep}}(\varepsilon) = \frac{4\pi k_b T}{\hbar} \sum_{kk'} |M(k,k')|^2 \frac{q^2}{\hbar \omega(k-k')} \delta(\varepsilon(k) - \varepsilon(k')). \quad (6)$$

The following approximations were introduced: $\hbar \omega >> k_b T$ permits phonon
occupation factors to be replaced by \( \frac{k_B T}{\hbar \omega} \); similarly, the fact that thermal electrons typically have energies a lot bigger than phonons permits the energy conserving delta functions to omit the energy of the emitted or absorbed phonon; parabolic bands were assumed which allows the momentum relaxation factor to be replaced by

\[
(1 - \cos \theta) = \frac{q^2}{2k^2} \quad \text{where} \quad \vec{q} = \vec{k}' - \vec{k}.
\]

### B1. Deformation Potential (DP) scattering

Certain optic phonon modes have an electron-phonon matrix element \( M(k,k') \) which varies weakly with \((k,k')\) and can be replaced by \( M(0,0) \). Then the energy-dependent scattering rate is

\[
\frac{1}{\tau_{DP}(\epsilon)} = \frac{2\pi k_B T}{\hbar} N_c(\epsilon) \Phi_{DP} \propto T \epsilon^{1/2}
\]

The coupling constant \( \Phi_{DP} \) is found from density-functional theory using

\[
\Phi_{DP} = \sum_{\alpha \beta} \langle 0 | \nabla_{\alpha \beta} V | 0 \rangle \left( K^{-1} \right)_{\alpha \beta} \langle 0 | \nabla_{\beta \alpha} V | 0 \rangle,
\]

where \( |0\rangle \) is the Bloch state with \( k = 0 \) at the bottom of the conduction band. Only the 6 phonons with \( A_{1g} \) symmetry have non-zero matrix elements coupling the \( k = 0 \ A_{1g} \) state to itself. This allows the matrix element to be written

\[
\Phi_{DP} = \sum_{\lambda} \frac{\Xi_\lambda^2}{\omega_\lambda'^2}
\]
where the modes $\lambda$ are the $A_{1g}$ phonons, and the deformation potentials $\Xi_\lambda$ are the normalized rates of shift of the energy $\epsilon_c(k = 0)$ of the conduction band bottom per unit displacement of modes $\lambda$. Averaging and evaluating, we get

$$
\frac{\hbar}{\langle \tau_{\text{Dr}}(T) \rangle} = \frac{3\sqrt{\pi}}{4} \frac{\hbar}{\tau_{\text{Dr}}(\epsilon = k_B T)} = 0.068 \text{eV} \left(\frac{T}{10^4 \text{K}}\right)^{3/2}
$$

(10)

**B2. Fröhlich (F) scattering**

Certain phonon modes are optically active because they create local electrical polarization. Their energy-dependent scattering rates (with $k = \sqrt{2m\epsilon / \hbar^2}$) is

$$
1/\tau_{\text{F}}(\epsilon) = \frac{2\pi}{\hbar} N_c(\epsilon) \left(\frac{4\pi Z^* \epsilon^2}{\Omega_c \epsilon_{\text{c},c}}\right)^{1/2} \frac{k_B T}{4M^* \omega_{\text{LO}}^2} G(b) \propto T \epsilon^{-1/2}
$$

(11)

The volume $\Omega_u = \Omega_c/4$ refers to the volume for one SiO$_2$ unit, one fourth of the cell volume. There are actually 12 IR active modes which have oscillatory dipole moments. These have matrix elements which vanish for zero momentum transfer at $k = 0$, but rapidly increase with momentum transfer. Rather than calculate the coupling strength to each of these twelve, we instead think of an alternate basis spanning the 36-dimensional displacement space of the 12 atoms in the unit cell. Let three of the spanning vectors be center of mass conserving displacements with each Si atom having equal displacement in one spatial direction parallel or perpendicular to $q$, and each oxygen displacing in the
opposite direction. This vector has maximum polarity, and the 33 orthogonal vectors carry no dipole moment. The one of these three vectors parallel to $q$ couples strongly by the Fröhlich mechanism to electrons near $k = 0$, scattering them to $k+q$ by the screened Coulombic dipole interaction. This vector is not an eigenstate, but is a superposition of the 12 polar eigenstates, composed primarily of the highest energy polar modes. We assign to this vector an energy equal to the average of the energies ($\hbar \omega_{k,LO} = 0.21eV$) of the most energetic polar mode in each of the $x$, $y$, and $z$ directions. The effective charge $Z^*$ of silicon is not known exactly, but is reduced from the formal charge of 4. We take it to be 2. The reduced mass $M^*$ for this “pseudo-LO” phonon mode is

$$\frac{1}{M^*} = \frac{1}{M_{Si}} + \frac{1}{2M_{O}}. \quad (12)$$

The factor $G(b)$ is the correction for Debye-Hückel screening of the Coulomb field of the polar LO phonon mode. This factor is defined as

$$G(b) = \frac{\sum_q \left( \frac{q^2}{q^2 + \kappa^2} \right)^2 \delta(\epsilon_{k+q} - \epsilon_k)}{\sum_q \delta(\epsilon_{k+q} - \epsilon_k)} = 1 - \frac{2}{b} \log(1 + b) + \frac{1}{1 + b}, \quad (13)$$

where $\kappa$ is the inverse Debye-Hückel screening length

$$\kappa^2 = \frac{4\pi e^2}{\epsilon_\infty} \frac{n}{k_B T} \approx 0.23 a_B^{-2} \left( \frac{10^4 K}{T} \right)^{1/4} e^{-E_g/2k_B T} \quad (14)$$
and $b$ is defined as

$$b = (2k / \kappa)^2. \quad (15)$$

The integral for thermal averaging, Eq. 5, is complicated because of the screening function $G(b)$. However, this function is slowly varying and can be approximated by its value when the rest of the integrand is maximum, namely at $\varepsilon = 2k_B T$. Then $G(b_{\text{max}}) \approx 0.64$ at $T = 10^4 K$, showing that screening reduces the Fröhlich scattering only moderately. The averaged Fröhlich scattering is then

$$\hbar / \langle \tau_F (T) \rangle = \frac{3\sqrt{\pi}}{8} \hbar / \tau_F (\varepsilon = k_B T) = 0.08 \text{eV} \left( \frac{T}{10^4 K} \right)^{1/2}. \quad (16)$$

**B3. Impurity (imp) scattering**

The formula for incoherent scattering from a total of $N_{\text{imp}}$ screened charged impurities, in Born approximation, is

$$1 / \tau_{\text{imp}}(\vec{k}) = \frac{2\pi}{\hbar} N_{\text{imp}} \sum_{k} \left( \frac{4\pi Z_{\text{imp}} e^2}{\Omega \varepsilon_{\text{imp}} \left( [\vec{k} - \vec{k'}]^2 + \kappa^2 \right)} \right)^{1/2} \left( \frac{\varepsilon - \varepsilon_{\text{imp}}}{2k^2} \right) \delta(\varepsilon - \varepsilon_{\text{imp}}), \quad (17)$$

where $Z_{\text{imp}}$ is the effective charge of the impurity, for example, nominally -1 if an Al$^{3+}$ ion occupies an Si$^{4+}$ site, and $\Omega$ is the volume of the sample. The formula can be written as
\[
1/\tau_{\text{imp}}(\varepsilon) = \frac{\pi x_{\text{imp}} N_{\nu}(\varepsilon) \left( \frac{4\pi Z_{\text{imp}}e^2}{\Omega_x\varepsilon_xk^2} \right)^2 F(b)}{h} \propto \varepsilon^{-3/2}, \quad (18)
\]

where \(x_{\text{imp}}\) is the fraction of Si atoms replaced by impurities. The factor \(F(b)\) is the correction for Debye-Hückel screening of the Coulomb field of the charged impurity.

This factor is defined as
\[
F(b) = \frac{\sum_q \left( \frac{q^2}{q^2 + k^2} \right)^2 \left( \frac{2k}{q} \right)^2 \delta(\varepsilon_{k+q} - \varepsilon_{k})}{\sum_q \delta(\varepsilon_{k+q} - \varepsilon_{k})} = \log(1+b) - \frac{b}{1+b}. \quad (19)
\]

This factor diverges in the \(b \to \infty\) weak screening limit, because the total bare Coulomb scattering cross section diverges. As in Fröhlich scattering, the thermal averaging integral is difficult because of the screening factor \(F(b)\), but \(F\) varies slowly with \(\varepsilon\) in the relevant range, so \(F\) can be replaced by its value at the point where the rest of the integral is maximized, namely \(\varepsilon = 3k_BT\). At \(10^4\) K, this gives \(F(h_{\text{max}}) \approx 2.26\).

The answer can now be written as
\[
\hbar/\left\{\tau_{\text{imp}}(T)\right\} = \frac{\sqrt{\pi}}{8} \hbar/\tau_{\text{imp}}(\varepsilon = k_BT) = 7.7x_{\text{imp}} \text{ eV} \left( \frac{T}{10^4\text{K}} \right)^{3/2} \quad (20)
\]

where the choice \(Z_{\text{imp}} = 1\) has been made.

**B4. Total Conductivity**

The correct procedure to get \(\sigma\) from Eq. 4 is to add the various energy-dependent
scattering rates from Eqs. 7, 11, and 18, take the reciprocal of this sum, and average according to Eq. 5. For simplicity we assume that one scattering mechanism, deformation potential scattering, is dominant. At \( T > 10^4 \) K, it exceeds Fröhlich scattering. Impurity scattering may be even more important, but brings additional complications.

Insulating rocks at temperatures \( T \leq 2000 \) K in the earth's mantle do not have many thermal carriers. Electrical conduction then occurs through complicated defect-mediated processes, such as electron hopping [21] from \( \text{Fe}^{2+} \) to \( \text{Fe}^{3+} \). Such processes are still available at \( 10^4 \) K, but are swamped by thermal carrier drift in the conduction band. The solubility and valence state of Fe impurities in cotunnite-type SiO\(_2\) is a complicated issue remaining to be investigated. Almost certainly the MgO phase attracts more of the Fe impurities than the SiO\(_2\) phase. Impurities which can change their ionization state allow a cheaper source of free carriers than does intrinsic thermal excitation across the insulating gap. Suppose the concentration \( x_{\text{imp}} \) of ionized impurities were 10\%. Then impurity scattering would be larger by 5 at \( 10^4 \) K (but diminishing with \( T \)) than intrinsic electron-phonon scattering. At the same time, the carrier density might well be
increased by a corresponding factor of 5.

For simplicity, we now ignore impurities and estimate the intrinsic conductivity of hot cotunnite-type SiO$_2$. Adding deformation potential and Fröhlich scattering, at 10$^4$ K the average $\langle \tau(T) \rangle$ is $\hbar/0.15$ eV (summing Eqs. 10 and 16). The thermal average has not been done correctly, but the error is not large. The total conductivity is then

$$\sigma = (4.8 \times 10^4 \Omega^{-1} \text{cm}^{-1}) \left( \frac{T}{10^4 \text{K}} \right)^{3/4} e^{-E_g/2 \hbar T}$$

which gives the result $\sigma = 2.6 \times 10^3 \Omega^{-1} \text{cm}^{-1}$ used in the main text.

**B5. Literature**

Not all the equations given here can be found in the literature. The averaging formula Eq. 5 is found in all texts in some form, specifically Refs. S14 (p.423), S15 (p.256), S16 (p.129), and S17 (p.106). The results for ionized impurity scattering, Eqs. 18 and 20, are standard and can be found in Refs. S16 (Ch.4), S15 (p.179), and S17 (p.131). Our approximate treatment of the thermal average of $F(b)$ is mentioned by Blatt in Ref. S15 (p.257).

The results for electron-phonon scattering in the literature are often more complicated than our results, Eqs. 7 and 11. The reason for comparative simplicity in
our case is the high $T$ approximation which allows the energy conserving delta functions to contain only the electron energy. Dropping the phonon energy is equivalent to approximating the scattering as elastic which is a good approximation if the electron energy is a few times larger than the phonon energy. The temperature averaged results Eqs.10 and 16 are equivalent to results obtained in the high $T$ limit in Refs. S14 (pp.437,439) and S15 (p.257 for Fröhlich scattering). Our Eqs. 8 and 9 are generalizations to complex unit cells of the standard ideas of optical deformation potentials.

C. Thermal conductivity

C1. Electronic heat conduction

In semiconductors, electronic thermal conductivity is usually swamped by the vibrational part, whereas in metals, the reverse is often true. High $T$ cotunnite-type SiO$_2$ is like a metal in this respect. The Wiedemann-Franz law gives the proportionality between electrical ($\sigma$) and thermal ($\kappa$) conductivity [S15],

$$\frac{\kappa_{el}}{\sigma_{el}} = \frac{k_B T}{e^2} \left( \frac{5}{2} + q \right)$$

(22)

where $q$ is the power law of the energy dependence of the electron scattering time.
\( \tau(\varepsilon) \propto \varepsilon^\eta \). Again, we assume that the dominant mechanism is deformation potential scattering, giving \( q = -1/2 \). This yields the result

\[
\kappa_{el} = \left( 7.1 \times 10^2 \, \text{W/mK} \right) \left( \frac{T}{10^4 \, K} \right)^{1/4} e^{-E_e/2k_B T} \tag{23}
\]

which yields the value 40W/mK used in the text.

**C2. Radiative heat conduction**

Radiation in transparent media gives ballistic heat transport, properly distinguished from conductive heat transport. However, a large medium like the earth is never transparent, and electromagnetic radiation should be regarded as an additional conductive channel, with photons rather than phonons or electrons providing the carrier. Black body energy density increases as \( T^4 \), and photon mean free paths are often many photon wavelengths, so barring absorptive mechanisms, radiation will eventually dominate \( \kappa(T) \). However, free charge carriers interact very strongly with light, giving essentially no propagating photons of frequency less than the metallic plasma frequency,

\[
\omega_p = \sqrt{4 \pi n e^2 / \varepsilon_in} \ . \text{ Our estimate is}
\]

\[
\hbar \omega_p = (3.7 \text{eV}) \left( \frac{T}{10^4 \, K} \right)^{3/8} e^{-E_e/4k_B T} \tag{24}
\]

or \( \hbar \omega_p \approx 0.9 \text{eV} \) at \( 10^4 \) K. Thus radiative heat transport is shut down for photons of
energy less than 0.9 eV. At higher energies, allowed photon absorption from mid-gap energy levels of even dilute impurities will probably diminish $\kappa_{\text{rad}}$ considerably.

**Supporting Online Figures**

![Graphs showing logarithmic derivatives of magnesium at 1.6 a.u., silicon at 1.4 a.u., and oxygen at 1.2 a.u.](image)

**Fig. S1** Logarithmic derivatives of magnesium at 1.6 a.u., silicon at 1.4 a.u., and oxygen at 1.2 a.u. Thin solid and bold dashed lines are logarithmic derivatives of all-electron and pseudo wave functions, respectively.
Fig. S2A Phonon dispersions of CaIrO$_3$-type MgSiO$_3$. 
Fig. S2B Phonon dispersions of CsCl-type MgO. Red arrows point to imminent soft mode instability.
**Fig. S2C** Phonon dispersions of cotunnite-type SiO$_2$. Red arrows point to imminent soft mode instability.
Fig. S3  Pressure-density relations of CaIrO$_3$-type MgSiO$_3$ and the aggregation of CsCl-type MgO and cotunnite-type SiO$_2$ at several temperatures. Discontinuities in these lines correspond to the density increase at dissociation (Fig. 3B).
Fig. S4 Metastable ultra high $PT$ structures of MgSiO$_3$ found at 12 Mbar.
Table S1 Comparison between calculated (Birch-Murnaghan) and experimental equations of state parameters for NaCl-type MgO and stishovite. This comparison is a direct test of the accuracy of the current pseudopotentials.

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<th>( B'_0 )</th>
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Table S2 Density profiles of CaIrO$_3$-type MgSiO$_3$ and the aggregation of CsCl-type MgO and cotunnite-type SiO$_2$. Densities are in g/cm$^3$.

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References for Supporting Online Material


