ARE SILICON NANOPARTICLES AN INTERSTELLAR DUST COMPONENT?

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ABSTRACT

Silicon nanoparticles (SNPs) with oxide coatings have been proposed as the source of the observed “extended red emission” (ERE) from interstellar dust. We calculate the thermal emission expected from such particles, both in a reflection nebula such as NGC 2023 and in the diffuse interstellar medium (ISM). It is shown that Si/SiO₂ SNPs (both neutral and charged) would produce a strong emission feature at 20 µm. The observational upper limit on the 20 µm feature in NGC 2023 imposes an upper limit of less than 0.2 parts per million in Si/SiO₂ SNPs. The observed ERE intensity from NGC 2023 then gives a lower bound on the product, η_PL f₀, where η_PL < 1 is the photoluminescence efficiency for a neutral SNP and f₀ ≤ 1 is the fraction of SNPs that are uncharged. For foreground extinction A₀.68 µm = 1.2 mag, we find η_PL f₀ > 0.24 for Si/SiO₂ SNPs in NGC 2023. Measurement of the R-band extinction toward the ERE-emitting region could strengthen this lower limit. The ERE emissivity of the diffuse interstellar medium appears to require ≥42% of solar Si abundance in Si/SiO₂ SNPs even with η_PL f₀ = 1. We predict IR emission spectra and show that DIRBE photometry appears to rule out such high abundances of free-flying SNPs in the diffuse ISM. We conclude that if the ERE is due to SNPs, they must be either in clusters or attached to larger grains.

Subject headings: dust, extinction — infrared: ISM — ISM: individual (NGC 2023) — ISM: lines and bands — reflection nebulae

1. INTRODUCTION

First detected in the Red Rectangle (Schmidt, Cohen, & Margon 1980), “extended red emission” (ERE) from interstellar dust consists of a broad, featureless emission band between ~5400 and 9000 Å, peaking at 6100 Å ≤ λg ≤ 8200 Å and with a width 600 Å ≤ FHWM ≤ 1000 Å. The ERE has been seen in a wide variety of dusty environments: the diffuse interstellar medium (ISM) of our Galaxy, reflection nebulae, planetary nebulae, H II regions, and other galaxies (see Witt, Gordon, & Furton 1998 for a summary). The ERE is generally attributed to photoluminescence (PL) by some component of interstellar dust, powered by ultraviolet (UV)/visible photons. The photon conversion efficiency of the diffuse ISM has been determined to be near 10% ± 3% (Gordon, Witt, & Friedmann 1998; Szomoru & Guthakurta 1998), assuming that all UV/visible photons absorbed by interstellar grains are absorbed by the ERE carrier. The actual photoluminescence efficiency η.PL of the ERE carrier must exceed ~10%, since the ERE carrier cannot be the only UV/visible photon absorber.

Various forms of carbonaceous materials—hydrogenated amorphous carbon (Duley 1985; Witt & Schild 1988), polycyclic aromatic hydrocarbons (PAHs; d’Hendecourt et al. 1986), quenched carbonaceous composite (Sakata et al. 1992), C₄₀₀ (Webster 1993), coal (Papoular et al. 1996), PAH clusters (L. J. Allamandola 2001, private communication), and carbon nanoparticles (Seahra & Duley 1999)—have been proposed as carriers of ERE. However, most candidates appear to be unable to simultaneously match the observed ERE spectra and the required PL efficiency (see Witt et al. 1998 for details).

It is worth noting that high photoluminescence efficiencies can be obtained by PAHs. Arguments against PAHs as ERE carriers include (1) the presence of sharp structures in the luminescence spectra of individual PAH molecules, in contrast to the featureless nature of the interstellar ERE spectra; (2) the lack of spatial correlation between the ERE and the PAH IR emission bands in the compact H II region Sh 152 (Darbon et al. 2000), the Orion Nebula (Perrin & Sivan 1992), and the Red Rectangle (Kerr et al. 1999); (3) ERE detection in the Bubble Nebula, where no PAH emission has been detected (Sivan & Perrin 1993); and (4) nondetection of ERE emission in reflection nebulae illuminated by stars with effective temperatures T_eff ≤ 7000 K (Darbon, Perrin, & Sivan 1999), whereas PAH emission bands have been seen in such regions (e.g., see Uchida, Sellgren, & Werner 1998) and are expected for the PAH emission model (A. Li & B. T. Draine 2001, in preparation). Argument (1) may not be fatal since a featureless band may result from a mixture of many individual PAH molecules and ions.

We also note that Seahra & Duley (1999) argued that small carbon clusters were able to meet both the ERE profile and the PL efficiency requirements. However, this hypothesis appears to be ruled out by nondetection in NGC 7023 of the 1 µm ERE peak (Gordon et al. 2000) predicted by the carbon nanoparticle (CNP) model. More recently, Duley (2001) further argued that the CNP model, which suggests that CNPs are responsible for both the PAH bands and the ERE, is supported by the lack of correlation between the 3.3 µm PAH band and the ERE intensity because particles with high photoluminescence efficiencies are not heated sufficiently to radiate significantly at 3.3 µm. However, this does not readily explain the fact that the ERE intensity does not correlate with the PAH bands at longer wavelengths (e.g., see Darbon et al. 2000).

Very recently, Witt et al. (1998) and Ledoux et al. (1998) suggested crystalline silicon nanoparticles (SNPs) with 15–50 Å diameters as the carrier on the basis of experimental data showing that SNPs could provide a close match to the observed ERE spectra and satisfy the quantum efficiency requirement. It was estimated by Witt et al. (1998) and Ledoux et al. (1998) that SNPs account for ≤5% of the total interstellar dust mass, with Si/H ≈ 6 parts per million.
that the typical core size should be
as discussed below, the observed ERE spectrum indicates
with density \( g_{\text{SiO}_2} \) (Grevesse & Sauval 1998).

More recently, Smith & Witt (2001) have further developed
the SNP model for the ERE, concluding that the observed
ERE in the diffuse ISM can be explained with
\( \text{Si}/H = 6 \text{ ppm} \) in \( \text{SiO}_2 \)-coated SNPs with Si core radii
\( a \approx 17.5 \text{ Å} \).

The purpose of this paper is to test the SNP hypothesis.
We calculate the IR spectra for SNPs in a reflection nebula—NGC 2023—and compare with observations. We show that the SNPs in NGC 2023 contain \( \text{Si}/H \leq 0.2 \text{ ppm} \). We reestimate the minimum Si depletion in SNPs required to account for the observed ERE intensity in the diffuse ISM and calculate the IR emission expected from such particles. We show that existing DIRBE photometry appears to rule out the abundances of free-flying SNPs required to account for the ERE emissivity of the diffuse ISM. Future observations by the Space Infrared Telescope Facility (SIRTF) will be even more sensitive to the abundance of SNPs in the diffuse ISM.

In § 2 we discuss the optical properties and heat capacities of Si/\( \text{SiO}_2 \) nanoparticles. In § 3 we carry out calculations for the IR emission spectra of SNPs and discuss their implications. In § 4 we discuss the effects of mantle thickness and grain shape and sources of uncertainties. Our conclusions are presented in § 5.

2. GRAIN PHYSICS

2.1. Composition

Experimental studies indicate that high photoluminescence efficiencies are observed from Si nanocrystals only when their surfaces have been “passivated” by oxidation or hydrogenation—otherwise, electron-hole pairs recombine nonradiatively (see, e.g., Kovalev et al. 1999). Accordingly, SNPs with oxide coatings are likely to be of primary interest as the source of the ERE. Pure Si SNPs will therefore not be considered here. Readers interested in the IR emission spectra of pure Si SNPs are referred to Li & Draine (2001a).

The Si core is assumed to be crystalline, with density \( \rho_{\text{Si}} \approx 2.4 \text{ g cm}^{-3} \), and the oxide mantle is assumed to have the properties of glassy \( \text{SiO}_2 \), with density \( \rho_{\text{SiO}_2} \approx 2.2 \text{ g cm}^{-3} \). We will consider core radii \( a_{\text{Si}} \) in the range 10–50 Å. As discussed below, the observed ERE spectrum indicates that the typical core size should be \( a_{\text{Si}} \approx 17.5 \text{ Å} \).

A single monolayer of \( \text{SiO}_2 \) would have a thickness \( \Delta a \approx (60m_{\text{HI}}/\rho_{\text{SiO}_2})^{1/3} \approx 3.6 \text{ Å} \), where \( m_{\text{HI}} \) is the mass of a hydrogen atom. In the laboratory, Si nanocrystals exposed to air spontaneously form an overlayer of \( \text{SiO}_2 \) that is \( \approx 10 \text{ Å} \) thick (Ledoux et al. 1998). Witt et al. (1998) propose that interstellar SNPs form from \( \text{SiO}_2 \) in stellar outflows, with subsequent separation of 50% of the Si atoms into a crystalline Si core and the remaining 50% in an \( \text{SiO}_2 \) mantle; for this case the mantle thickness would be \( \Delta a \approx 0.49a_{\text{Si}} \approx 8.6 \text{ Å} (a_{\text{Si}}/17.5 \text{ Å}) \).

The oxide thickness expected under interstellar conditions is uncertain, but “passivation” presumably requires at least one monolayer of oxide. For the Si core radius \( a_{\text{Si}} \approx 17.5 \text{ Å} \) indicated by the ERE spectrum (Smith & Witt 2001), this would correspond to \( a_{\text{Si}}/a \approx 0.8 \), where \( a \) is the overall grain radius.\(^1\) For most of the calculations reported here, we will assume \( a_{\text{Si}}/a = 0.8 \), with the core containing 51% of the volume and 71% of the Si atoms and with the mantle thickness corresponding to approximately one monolayer of \( \text{SiO}_2 \) for the typical radius \( a_{\text{Si}} = 17.5 \text{ Å} \). However, to illustrate the insensitivity of the calculated IR emission spectrum to the actual \( \text{SiO}_2 \) mantle thickness, we will also show IR spectra for SNPs with 90% of the Si atoms in the core, or \( a_{\text{Si}}/a = 0.926 \) (see § 4).

2.2. Optical Properties

The optical properties of crystalline Si nanoparticles are uncertain. Some studies (see Yoffe 2001 for a recent review) have concluded that the optical properties of Si nanoparticles differ substantially from those of bulk Si. This has been attributed to the quantum confinement effect (Wang & Zunger 1994; Tsu, Bubic, & Ioriatti 1997). Koshiba et al. (1993; hereafter K93) have published dielectric constants for crystalline nanosilicon that are considerably smaller than those of bulk Si. We find that the absorption and reflectivity measurements for porous silicon (e.g., K93; de Filippo et al. 2000) appear to be inconsistent with the K93 optical constants;\(^2\) instead, they can be approximately reproduced using a mixture of Si and voids, if the Si component is described using the optical constants of bulk Si, as previously found by Kovalev et al. (1996), Theiss (1997), Léondel et al. (2000), and Diesinger, Bsiyes, & Hérino (2001). Oxide layers are generally also present in laboratory samples of porous Si; we find that the measured absorption and reflectance spectra can also be satisfactorily reproduced using Bruggeman effective medium theory (Bohren & Huffman 1983) for a mixture of voids, \( \text{SiO}_2 \), and bulk Si.

We take the following “synthetic” approach to obtain the complex refractive index \( m(\lambda) = m' + i m'' \) for bulk Si at low temperatures, with no electron-hole pairs present (the contribution of electron-hole pair pairs will be treated separately). For 0.01 \( \mu \text{m} < \lambda < 1.2 \mu \text{m} \), we take \( m''(\lambda) = 2.4 \times 10^{-8} \) estimated from the (room temperature) absorption coefficient \( \alpha \approx 10^{-3} \text{ cm}^{-1} \) of bulk Si between 1 and 3 \( \mu \text{m} \) (Gray 1972). For 3.6 \( \mu \text{m} < \lambda < 25 \mu \text{m} \), we take those of Palik (1985) for crystalline bulk Si; extrapolation is then made for \( \lambda > 25 \mu \text{m} \).\(^3\) After smoothly joining the adopted \( m'' \), we calculate \( m' \) from \( m'' \) through the Kramers-Kronig relation (Bohren & Huffman 1983, p. 28).

The Si long-wavelength absorption properties will depend on whether any free electrons or holes are present. SNPs are thought to luminesce only when uncharged and

\(^1\) This thickness is also consistent with some experimental studies that show that the oxidation of the Si core is a self-limiting process and, in the final stage of oxidation, the thickness of the oxide layer represents about 20% of the total particle radius (Ledoux et al. 2000).

\(^2\) For example, the calculated absorption coefficient and reflectivity based on the K93 optical constants and assuming a mixture of voids (70% by volume; see K93; de Filippo et al. 2000), Si, and \( \text{SiO}_2 \) (with various Si/\( \text{SiO}_2 \) volume ratios) are significantly lower than the experimental values.

\(^3\) We do not adopt those of Palik (1985) for \( \lambda > 25 \mu \text{m} \) since they were measured at \( T \approx 300 \text{ K} \) and the \( \lambda > 25 \mu \text{m} \) absorption is dominated by thermally excited electron-hole pairs. To estimate the dielectric function in the absence of such pairs, we approximate \( m''(\lambda) \approx m''(25 \mu \text{m}/25 \mu \text{m}/25 \mu \text{m}) \). The IR bands of Si nanoparticles may become stronger because of the symmetry-breaking surfaces (e.g., see Hölstein et al. 2000). New IR bands, forbidden in bulk Si, may also appear (S. Adachi 2001, private communication). Unfortunately, IR measurements of Si nanoparticles are unavailable, so we must use the optical properties of bulk Si.
containing exactly one electron-hole pair, which recombines radiatively in ~10^{-3} s (Smith & Witt 2001). The thermal energy remaining after luminescence will then be radiated by a SNP with no free electrons or holes. Electron-hole recombination occurs more rapidly than radiative cooling, so for purposes of calculating the infrared emission, we assume a neutral SNP to contain no electrons or holes and charged SNPs to contain only free electrons (if negative) or holes (if positive). The contribution of free electrons or holes to the dielectric function is approximated by

$$\delta \varepsilon \approx \frac{-(\omega_p \tau)^2}{(\omega_p \tau)^2 + i\omega \tau},$$  

(1)

and

$$\omega_p^2 = \frac{3|Z| \epsilon^2}{4\pi a_{Si}^3 4\pi m_{eff}},$$  

(2)

where \(\omega\) is the frequency, \(\omega_p\) is the plasma frequency, \(\tau\) is the collision time, \(Ze\) is the grain charge, \(a_{Si}\) is the Si core radius, \(m_{eff}\) is the effective mass of a free electron or hole, and \(e\) is the proton charge. We adopt an effective mass \(m_{eff} \approx 0.2 m_e\) for electrons or holes in Si.\(^4\) Scattering by the Si boundary will result in a collision time \(\tau \approx a/v_F\), where we take \(v_F \approx 10^8\) cm s^{-1} as the typical velocity.\(^5\)

In Figure 1 we plot the resulting optical constants for crystalline SNPs, for both neutral SNPs and SNPs with a radius \(a = 10\) Å and a charge \(Z = \pm 1\). We see that the hole dominates the absorption for \(\lambda \gtrsim 1\) μm and completely overwhelms the weak vibrational bands in the 7–25 μm region, which provide the infrared absorption in neutral Si. For comparison, we also show the optical constants from K93.

For glassy SiO\(_2\), we take \(m''\) from Palik (1985) for 0.01 μm \(< \lambda < 7\) μm, but with one modification: for 0.15 μm \(< \lambda < 3.6\) μm, we set \(m'' = 1.0 \times 10^{-4}\) based on the absorption coefficient measured by Harrington, Rudisill, & Braunstein (1978). For 7 μm \(< \lambda < 500\) μm, we take \(m''\) from Henning & Mutschke (1997) for a glassy SiO\(_2\) sample at 100 K (the optical properties of glassy SiO\(_2\) are not sensitive to temperature; see Henning & Mutschke 1997). For \(\lambda > 500\) μm, we approximate \(m''(\lambda) \approx m''(500\) μm)/500 μm/λ). Again, the real part \(m'\) is calculated from the Kramers-Kronig relation. The results are also presented in Figure 1.

In Figure 2 we show the absorption cross sections per unit volume calculated for both spherical and randomly oriented spheroidal (a) pure Si grains and (b) Si/SiO\(_2\) grains, with the Si in a confocal spheroidal core containing a fraction (0.8)\(^3\) = 51% of the volume. For spherical grains we use the exact series expansions for coated spheres (Bohren & Huffman 1983); for spheroidal grains we use the electric-dipole or Rayleigh approximation (Draine & Lee 1984), which is valid since \(a/\lambda \ll 1\) for \(a < 60\) Å and \(\lambda > 912\) Å. We also plot in Figure 2c the radiation fields for the diffuse ISM and for NGC 2023 (60° south of HD 37903; see § 3.1).

Figures 2a and 2b clearly show that in the wavelength range where Si or Si/SiO\(_2\) grains absorb most (λ \(< 0.25\)

\(^4\) For a positively charged SNP, the relevant mass is the effective mass of a hole. There are two degenerate valence band maxima, with hole masses 0.49\(m_e\) and 0.16\(m_e\) (Ashcroft & Mermin 1976, p. 569); we adopt 0.2\(m_e\) as a representative value. The conduction band minima are characterized by electron effective masses of 1.0\(m_e\) and 0.2\(m_e\); these would be relevant for negatively charged SNPs.

\(^5\) Our estimate of \(\tau\) is by no means exact, but we will see below that the value of \(\tau\) is unimportant in the case of oxide-coated SNPs, since the oxide layer dominates the IR emission.
The mean absorption cross section per unit volume $C_{abs}/V$ weighted by the $\lambda < 5500$ Å starlight intensity $cu_\lambda/4\pi$, 

$$\langle C_{abs}/V \rangle \approx \int_{5500\text{Å}}^{\infty} \left[ C_{abs}(\lambda)/V \right] cu_\lambda d\lambda,$$

is a frequently used quantity in studies of the photophysics of the ERE carrier. In the diffuse ISM ($\int_{912\text{Å}}^{\infty} cu_\lambda d\lambda \approx 6.2 \times 10^{-2}$ ergs cm$^{-2}$s$^{-1}$), we find $\langle C_{abs}/V \rangle \approx 8.9 \times 10^4$ cm$^{-1}$ for the interstellar dust model of Weingartner & Draine (2001) for $R_V = 3.1$. We find $\langle C_{abs}/V \rangle \approx 5.8 \times 10^5$ cm$^{-1}$ for pure Si nanoparticles and $\langle C_{abs}/V \rangle \approx 3.2 \times 10^5$ cm$^{-1}$ for Si/SiO$_2$ nanoparticles with $a_{Si} = 0.8a$.

2.3. Enthalpies

The experimental specific heat of bulk crystalline Si (Touloukian & Buyco 1970a) can be approximated by a Debye model with dimensionality $n = 3$ and Debye temperature $\Theta = 530$ K, while SiO$_2$ glass (Touloukian & Buyco 1970b) can be approximated by a model where one-third of the vibrational modes are distributed according to a Debye model with $\Theta = 275$ K and two-thirds of the modes according to a Debye model with $\Theta = 1200$ K.

For very small particles at low temperatures, the discrete nature of the vibrational spectrum becomes important. Let $N_{Si}^{atom}$ and $N_{SiO_2}^{atom}$ be the number of atoms in the Si core and SiO$_2$ mantle and $N_{atom} = N_{Si}^{atom} + N_{SiO_2}^{atom}$ be the total number of atoms. For pure Si clusters, we set $N_m = 3N_{Si}^{atom} - 6$ vibrational modes, where the “6” term allows for the translational and rotational degrees of freedom since the energy from photon absorption is distributed only among the vibrational modes. For Si/SiO$_2$ nanoparticles, we assume $N_m = 3N_{Si}^{atom} - 3$ modes distributed according to a $\Theta = 530$ K Debye model, $N_m = 2N_{SiO_2}^{atom} - 2$ modes distributed according to a $\Theta = 1200$ K Debye model, and $N_m = N_{SiO_2}^{atom} - 1$ modes distributed according to a $\Theta = 275$ K Debye model. We assume the mode frequencies to be distributed following eqs. (4)−(6) and eq. (11) of Draine & Li (2001). The heat capacity $C(T)$ is calculated treating the modes as harmonic oscillators, with the continuum limit used for large particles and high energies (see Draine & Li 2001):

$$C(T) = 3(N_{Si}^{atom} - 1)k_f^2(T/\Theta_1) + 3(N_{SiO_2}^{atom} - 1)[(3/2)k_f^2(T/\Theta_2) + (5/12)k_f^2(T/\Theta_3)],$$

$$f_d(x) \equiv n \int_0^\infty \frac{y dy}{\exp(y/x) - 1}, \quad f_d(x) \equiv \frac{d}{dx} f_d(x),$$

where $k$ is the Boltzmann constant, $T$ is the grain vibrational temperature; the Debye temperatures $\Theta_1$, $\Theta_2$, and $\Theta_3$ are, respectively, 530, 275, and 1200 K. Note that there is a typographical error in the expression of $f_d(x)$ in equation (10) of Draine & Li (2001) and in equation (16) of Li & Draine (2001).

3. INFRARED Emission Spectrum and Its Implications

Let $Z_{Si}$ be the amount of Si in the grains (by number) relative to total hydrogen. The IR emissivity per unit solid angle per H nucleon from the SNPs is

$$j_\lambda(a) = \frac{Z_{Si}}{N_{Si}(a)} C_{abs}(a, \lambda) \int_0^\infty dT B_\lambda(T) P(a, T),$$

where $N_{Si} = \pi a_{Si}^3 \rho_{Si}/2m_n + \pi (a^3 - a_{Si}^3) \rho_{SiO_2}/4m_n$ is the number of Si atoms in a grain of radius $a$ for grains with Si cores of radius $a_{Si}$ and SiO$_2$ mantles, where $\rho_{Si}$ and $\rho_{SiO_2}$ are the mass densities of crystalline Si ($\approx 2.42$ g cm$^{-3}$) and glassy SiO$_2$ ($\approx 2.2$ g cm$^{-3}$), respectively, and $m_n$ is the mass of a hydrogen atom; $C_{abs}(a, \lambda)$ is the absorption cross section of the spherical core-mantle grain at wavelength $\lambda$, calculated using the optical constants discussed in § 2.2; $B_d(T)$ is the Planck function; and $P(a, T)$ is the emissivity of the grain temperature will be in $\langle T, T + dT \rangle$.

For a given radiation field, we calculate $P(a, T)$ for small grains employing the “thermal-discrete” method, which treats both heating (photon absorption) and cooling (photon emission) as discrete transitions, using a thermal approximation for the downward transition probabilities (Draine & Li 2001). We characterize the intensity of the illuminating starlight by $\chi$, the intensity at 1000 Å relative to the Habing (1968) radiation field. For NGC 2023, the spectrum is assumed to be a $22,000$ K dilute blackbody cutoff at the Lyman edge; for the diffuse interstellar medium, we take the spectrum of Mathis, Mezger, & Panagia (1983), with $\chi = 1.23$.

3.1. NGC 2023

The reflection nebula NGC 2023, at a distance $D = 450$ pc, is illuminated by the B1.5 V star HD 37903 ($T_{eff} = 22,000$ K, $L_*=7600$ $L_\odot$). A modest H II region surrounds the star, beyond which is a photodissociation region at an estimated distance $\sim 5 \times 10^{17}$ cm from the star. The radiation field is expected to have an intensity $\chi \approx 5000$ at this distance from the star. While $\chi \approx 5000$ is consistent with models to reproduce the observed IR and far-red emission from UV-pumped H$_2$ in the bright “emission bar” $80'$ south of HD 37903 (Draine & Bertoldi 1996, 2000), the integrated infrared 5–60 $\mu$m surface brightness at a position $60'$ south of HD 37903 (Fig. 4) points to a lower value of $\chi$. We will assume that the dust producing the measured infrared spectrum and ERE is illuminated by a radiation field with $\chi \approx 2000$.

The 2.4–45 $\mu$m spectrum has been obtained by Verstraete et al. (2001) using the Infrared Space Observatory (ISO), using apertures ranging from 14'’ × 20’’ (for 2.4–12 $\mu$m) to 20’’ × 33’’ (for 29–45 $\mu$m), at a position 60’’ south of HD 37903. Far-infrared photometry with a 37’’ beam centered 60’’ south of HD 37903 has been obtained from the Kuiper Airborne Observatory (KAO) by Harvey, Thronson, & Gatley (1980). The observed IR spectrum is shown in Figure 4. Proposed ERE carriers must not produce IR emission in excess of what is observed.

The photodissociation region (PDR) in NGC 2023 is optically thick to the illuminating starlight. Allowing for forward scattering, we estimate that the effective attenu-
From this we estimate the reflection region 60° south of HD 37903 (Witt & Boroson 1990, Fig. 4). The foreground extinction $A_k$ is uncertain. The line of sight to HD 37903 has $E(B-V) \approx 0.35$ mag and $R_v \equiv A_v/E(B-V) = 4.1$ (Cardelli, Clayton, & Mathis 1989), corresponding to $A_{0.68 \mu m} \approx 1.2$ mag. For the emission bar 80'' south of HD 37903, an extinction $A_{0.68 \mu m} \approx 3.2$ mag has been determined from the relative strengths of K-band and far-red H$_2$ emission lines (Draine & Bertoldi 2000). For purposes of discussion, we will assume that the extinction to the reflection region 60'' south of HD 37903 (where the ERE has been measured) is likely to be in the range 1.2 mag $\leq A_{0.68\mu m} \approx 3.2$ mag.

To estimate $f_{\text{ERE}}$ (= $\int I_\lambda^\text{ERE} \, d\lambda$) 60'' south of HD 37903, we take 1) the measured surface brightness profile from Witt, Schild, & Kraiman (1984, Fig. 7); 2) $I_{0.68 \mu m}/I_{0.62 \mu m} = 10^{0.06 \pm 0.08} \pm 0.91$ 80'' south of HD 37903, where $I_\lambda$ is the observed stellar flux (Witt & Schild 1988, Table 1); and 3) the ERE spectral profiles 62'' and 84'' east-northeast of HD 37903 (Witt & Boroson 1990, Fig. 4). From this we estimate $f_{\text{ERE}} \approx 9 \times 10^{-5}$ ergs cm$^{-2}$ s$^{-1}$ sr$^{-1}$ 60'' south of HD 37903. The ERE emissivity per H nucleon is

$$I_\lambda = \frac{N_H}{\cos \theta} j_\lambda 10^{-0.4A_k} \approx 4 \times 10^{21} \text{cm}^{-2} j_\lambda 10^{-0.4A_k},$$

where $A_k$ is the extinction between the point of emission and the observer.

We now calculate the temperature distribution functions $P(a, T)$ for Si/SiO$_2$ nanoparticles with $a_{Si} = 0.8$ Å (see § 2.1). Figure 4 presents $P(a, T)$ for both neutral and charged Si/SiO$_2$ SNPs of various sizes. As shown in Figure 3, the radiation field is so strong that grains with $a \gtrsim 30$ Å attain a steady-state temperature $\approx 96$ K. The single-photon heating effect (Greenberg 1968) is evident for $a_{Si} = 10$ Å.

We now calculate the IR emission spectra. In Figure 4 we show theoretical spectra for $a_{Si} = 10, 20, 30, 40,$ and 50 Å with $Z_{Si} = 15$ ppm (estimated in § 3.2 for Si/SiO$_2$ grains to account for the ERE in the diffuse ISM) together with the observed spectrum for NGC 2023. Results are shown for both neutral and charged SNPs; we see that the IR emission spectrum is essentially independent of whether the SNPs are neutral or charged.

The Si-O modes produce strong features at 20, 12.5, and 9.1 μm (see Fig. 4). The most conspicuous feature is the strong and broad 20 μm band, which, for $Z_{Si} = 15$ ppm, is $\sim 80$ times stronger than the observational data. To depress the 20 μm emission feature to a level not in contradiction with the observational spectrum, NGC 2023 must have $Z_{Si} \lesssim 0.2$ ppm in SiO$_2$-coated Si grains (all charge states).

Following Smith & Witt (2001), we assume that only neutral SNPs are able to luminesce. Let $\eta_{\text{PL}}$ be the photoluminescence efficiency for a neutral SNP, $\gamma_{Si}$ be the UV/visual photon absorption rate per Si atom (in the 912–5500 Å wavelength range), and $\langle h\nu \rangle_{\text{ERE}}$ be the mean energy of ERE photons. Since the NGC 2023 ERE peaks at $\approx 6800$ Å (Witt & Boroson 1990), we take $\langle h\nu \rangle_{\text{ERE}} \approx 1.8$ eV. Illuminated by starlight of $T_{eff} = 22,000$ K, we calculate $\gamma_{Si} \approx 6.19 \times 10^{-4} g(2000) s^{-1}$ Si$^{-1}$ for neutral Si/SiO$_2$ SNPs. If $f_{0}$ is the fraction of SNPs that are neutral, the ERE emissivity per H is

$$f_{\text{ERE}} = \langle h\nu \rangle_{\text{ERE}} \gamma_{Si} \eta_{\text{PL}} f_{0} Z_{Si}/4\pi \approx 1.42 \times 10^{-19} \eta_{\text{PL}} f_{0} Z_{Si} \text{ ergs s}^{-1} \text{sr}^{-1} \text{ H}^{-1}.$$  

From equation (8) we thus require $\eta_{\text{PL}} Z_{Si} \approx 1.62 \times 10^{-6} f_{0}^{1/2} 10^{0.4A_{0.68 \mu m}}$ for neutral Si/SiO$_2$ nanoparticles. For $A_{0.68 \mu m} = 1.2$ mag, the efficiency $\eta_{\text{PL}} \gtrsim 0.24 f_{0}^{-1}$. For $A_{0.68 \mu m} = 3.2$ mag, it is impossible for the SNP model to explain the observed ERE since the required $\eta_{\text{PL}} \gtrsim 1.54 f_{0}^{-1} > 150\%$.

The charge distribution expected for SNPs in NGC 2023 is uncertain but may be similar to the charge distribution expected for carbonaceous grains. Let $G$ be the ratio of the local 6–13.6 eV energy density relative to the estimate of

$$9 \text{ For Si/SiO}_2\text{-charged SNPs, we calculate a photoabsorption rate} \gamma_{Si} \approx 6.00 \times 10^{-5}(g/2000) \text{ s}^{-1} \text{Si}^{-1}, \text{ nearly the same as for neutral SNPs.}$$

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**Fig. 3.** Temperature distribution functions for Si/SiO$_2$ spheres of various radii, with the Si cores assumed to be (a) neutral and (b) charged with $Z = \pm 1$, for grains exposed to the radiation field in NGC 2023. Curves are labeled by the Si core radius $a_{Si}$ (≈ 0.8 Å where $a$ is the Si/SiO$_2$ radius).
charged, with \( f_0 \ll 1 \); one might expect SNPs to have similar rates for electron capture and photoelectron emission. While highly tentative, this estimate \( f_0 \ll 1 \) is troubling, because SNPs cannot account for the ERE in NGC 2023 unless either \( f_0 \gtrsim 0.25 \) (assuming \( \eta_{\text{PL}} = 100\% \) for neutral SNPs) or charged SNPs are able to luminesce.

We summarize the above results in Table 1.

### 3.2. Diffuse Interstellar Medium

Using Pioneer 10 and 11 observations, Gordon et al. (1998) estimated the ERE emissivity per H nucleon of the high Galactic latitude (HGL) diffuse ISM to be \( \langle f_{\text{ERE}} \rangle \approx 1.4 \times 10^{-26} \) ergs s\(^{-1}\) sr\(^{-1}\) H\(^{-1}\) ppm. Thus, \( \langle f_{\text{ERE}} \rangle \approx 1.04 \times 10^{-21} \langle \gamma / \gamma_{\text{H2}} \rangle \eta_{\text{PL}} f_0 Z_{\text{Si}} \) ergs s\(^{-1}\) sr\(^{-1}\) H\(^{-1}\) for Si/SiO\(_2\) grains. Therefore, since \( \eta_{\text{PL}} \lesssim 100\% \), we require \( Z_{\text{Si}} \gtrsim 15f_0^{-\frac{1}{2}} \) ppm \([\gtrsim 42\% \text{of (Si/H)}_0]\) for Si/SiO\(_2\) grains. In Figure 5 we plot the temperature probability distribution functions for these grains, and IR emission spectra are shown in Figure 6. Results are also summarized in Table 1.

Evidently, the DIRBE photometry rules out \( Z_{\text{Si}} \lesssim 15 \) ppm in Si/SiO\(_2\) nanoparticles (both neutral and charged) with radii \( a_{\text{Si}} \lesssim 35 \) Å. The DIRBE photometry places an upper limit \( Z_{\text{Si}} \lesssim 2 \) ppm on the abundance of the \( a_{\text{Si}} \approx 11 \) Å particle size, which appears to be required by the observed wavelength of peak emission in the diffuse ISM. Thus, we conclude that free-flying SNPs can account for no more than 13% of the observed ERE from the diffuse ISM, even if the neutral fraction \( f_0 \approx 1 \).

**SIRTF** will be able to obtain diffuse interstellar cloud emission spectra, which should either detect the 20 \( \mu \text{m} \) spec-

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**TABLE 1**

| ERE Emissivities of SNPs | NGC 2023 | Diffuse ISM |
|--------------------------|----------|-------------|
| **Observational** | | |
| \( \langle h\nu \rangle_{\text{ERE}} \) \( \text{ergs s}^{-1} \text{sr}^{-1} \) | 1.8 | 2.1 |
| \( \gamma_{\text{Si}} \) \( \text{sr}^{-1} \text{H}^{-1} \) \( \text{f}^{-1} \) | 2.3 \( \times 10^{-16} \) & 1.5 \( \times 10^{-16} \) |
| **Neutral Si/SiO\(_2\)** | | |
| \( \gamma_{\text{Si}} \) | 8.59 | 8.59 |
| \( \gamma_{\text{Si}} \) \( \text{ergs s}^{-1} \text{sr}^{-1} \text{H}^{-1} \) \( \text{f}^{-1} \) | 6.19 \( \times 10^{-16} \) & 3.87 \( \times 10^{-17} \) |
| **Charged Si/SiO\(_2\)** | | |
| \( \gamma_{\text{Si}} \) | 5.29 | 5.29 |
| \( \gamma_{\text{Si}} \) \( \text{ergs s}^{-1} \text{sr}^{-1} \text{H}^{-1} \) \( \text{f}^{-1} \) | 1.42 \( \times 10^{-15} \) & 1.04 \( \times 10^{-16} \) |

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For NGC 2023, \( \langle h\nu \rangle_{\text{ERE}} \) is estimated assuming a UV-illuminated slab with \( N_\text{H} = 2 \times 10^{21} \) cm\(^{-2}\) with limb-brightening \( 1/\cos \theta = 2 \) (see text).

The mean absorbed UV/visible photon energy \( \langle h\nu \rangle_{\text{abs}} \equiv \int f_{\nu} \lambda C_{\nu}(h\nu/c \nu) \Phi_{\nu}(h\nu/c \nu) \text{d}h\nu \), where \( c/\lambda \) is the starlight intensity.

The mean UV/visible photon absorption rate per Si atom \( \gamma_{\text{Si}} \equiv N_\text{Si} \int f_{\nu} \lambda C_{\nu}(h\nu/c \nu) \Phi_{\nu}(h\nu/c \nu) \text{d}h\nu \), where \( N_\text{Si} \) is the number of Si atoms in a SNP.

The model ERE emissivity per H nucleon \( \langle h\nu \rangle_{\text{ERE}} \equiv \langle h\nu \rangle_{\text{ERE}} \eta_{\text{PL}} f_0 Z_{\text{Si}}/4\pi \).
is responsible for the ERE), since the SiO₂ mantle is almost nonabsorptive for 0.12 \( \mu \text{m} \lesssim \lambda \lesssim 4 \mu \text{m} \); the core-mantle grains are cooled primarily by the SiO₂ mantle, since \( n' \) is so small for Si in the infrared (see Fig. 1). Therefore, increasing the amount of SiO₂ present (while holding the pure Si cores constant) will lead to only small changes in the IR emission resulting from the small decrease in average grain temperature (e.g., Si/SiO₂ grains with equal numbers of Si atoms in the core and in the mantle [\( a_{\text{Si}} \approx 0.668a \)] in NGC 2023 [\( \lambda = 2000 \)] have a steady-state temperature \( \approx 85 \text{ K} \) in comparison with \( \approx 96 \text{ K} \) for grains with \( a_{\text{Si}} = 0.8a \)). The limits on \( \eta_{\text{PL}} \) will be only slightly affected by increasing the thickness of the SiO₂ mantles.

On the other hand, for SNPs with a thinner SiO₂ mantle, the IR emission spectrum is still dominated by the 20 \( \mu \text{m} \) feature. For illustration, we show in Figure 7 the IR spectra calculated for a Si/SiO₂ grain with a much thinner SiO₂ mantle in NGC 2023 and the diffuse ISM (with \( a_{\text{Si}} = 17.5 \text{ Å} \) and \( a = 18.9 \text{ Å} \), the SiO₂ mantle contains \( \approx 21\% \) of the grain volume, in contrast to \( \approx 49\% \) for grains with \( a_{\text{Si}} = 0.8a \) as discussed above). It is seen that the resulting IR spectrum (for a given Si abundance) is very similar to that with a thicker SiO₂ mantle, except the grain with a thinner mantle is slightly hotter since the heating is dominated by the Si core. Therefore, we conclude that the SiO₂ mantle thickness does not affect our conclusion.

In §3 the grains are modeled as spherical. To investigate the sensitivity to shape variations, we have also calculated the IR emission spectra for (1) 5:1 prolate grains, (2) 5:1 oblate grains, and (3) grains with a distribution of spheroidal shapes with \( \Delta \rho / X = \Delta L \rho (L - 1)^{2} \) (Ossenkopf, Henning, & Mathis 1992), where \( 0 < L < 1 \) is the so-called depolarization factor parallel to the grain symmetry axis.
and the KAO photometry (conclusions are insensitive to the assumed grain shape. For core-mantle grains, we assume confocal geometry, with the above \( dP/dL = 0 \) (infinitely thin needles) or \( L_\parallel \rightarrow 1 \) (infinitely flattened pancake). For core-mantle grains, we assume confocal geometry, with the above \( dP/dL = 0 \) (infinitely thin needles) or \( L_\parallel \rightarrow 1 \) (infinitely flattened pancake). For core-mantle grains, we assume confocal geometry, with the above \( dP/dL = 0 \) (infinitely thin needles) or \( L_\parallel \rightarrow 1 \) (infinitely flattened pancake).

For neutral, (2) have an equivalent sphere-volume Si core size and illuminated by the NGC 2023 radiation field. All grains are taken to (1) be spheres and drops to zero for the extreme cases \( L_\parallel \rightarrow 0 \) (infinitely thin needles) or \( L_\parallel \rightarrow 1 \) (infinitely flattened pancake). For core-mantle grains, we assume confocal geometry, with the above \( dP/dL = 0 \) (infinitely thin needles) or \( L_\parallel \rightarrow 1 \) (infinitely flattened pancake). For core-mantle grains, we assume confocal geometry, with the above \( dP/dL = 0 \) (infinitely thin needles) or \( L_\parallel \rightarrow 1 \) (infinitely flattened pancake).

In a reflection nebula such as NGC 2023, the IR surface brightness due to SNPs \( \int \frac{dL}{d\lambda} \propto N_{\mathrm{H}} Z_{\mathrm{Si}}/\cos \theta \). While the fraction of the IR power radiated in the 20 \( \mu m \) SiO feature depends on \( \chi \) (through the grain temperature), this dependence is relatively weak for modest changes in \( \chi \). Therefore, the upper limit on the 20 \( \mu m \) feature in NGC 2023 gives an upper limit on \( N_{\mathrm{H}} Z_{\mathrm{Si}}/\cos \theta \); this limit, plus the observed ERE \( \propto \eta_{\mathrm{PL}} N_{\mathrm{H}} Z_{\mathrm{Si}}/\cos \theta \), then gives a lower limit on \( \eta_{\mathrm{PL}} \), independent of the actual values of \( N_{\mathrm{H}} \) and \( \cos \theta \) and only weakly dependent on the value of \( \chi \).

One considerable uncertainty in our analysis concerns the UV absorption properties of nano-Si material. In the literature, it is often stated that, as a result of quantum confinement, the optical-UV absorption of nano-Si is substantially reduced in comparison with that of bulk Si. If this is true, the SNP model would require an even larger Si abundance to account for the ERE, and the limitations placed on this model would be even more severe.

Another uncertainty concerns the IR emission properties of nano-Si crystals and nano-SiO\(_2\), which have not yet been experimentally investigated. In the present work, our results are mainly based on the IR optical properties of bulk Si and bulk SiO\(_2\). Nanomaterials are expected to be more IR active than their bulk counterparts (due to the symmetry-breaking surfaces), and therefore the detailed emission spectrum will be modified. Nevertheless, if the SNPs have an oxide coating, the very strong infrared-active O-Si-O bending mode at 20 \( \mu m \) is expected to dominate the IR emission from SNPs. The starlight energy absorbed by the grains has to be reradiated in the infrared, so the absence of detected spectral features will still place upper limits on the SNP abundance.

One may argue that nano-SiO\(_2\) material might have a broader 20 \( \mu m \) bending feature and a larger far-IR emissivity than those of bulk SiO\(_2\) adopted here (see Fig. 1 and § 2.2), due to the contributions of surface atoms. In the case of the diffuse ISM, our upper limit on \( Z_{\mathrm{Si}} \) is based on the broadband DIRBE photometry, which would be largely unaffected by moderate changes in the width of the 20 \( \mu m \) feature. In the case of NGC 2023, broadening of the 20 \( \mu m \) feature would lead to an increase in the upper limit on \( Z_{\mathrm{Si}} \) inferred from the observed spectrum, and therefore the observed ERE could be accounted for by a smaller value of \( \eta_{\mathrm{PL}} f_{\mathrm{O}} \). However, we note that existing experimental data of nanocrystals do not show any appreciable broadening of the IR vibrational bands (e.g., see Hofmeister, Rosen, & Speck 2000). We stress that accurate measurements of the optical properties of oxide-coated nano-Si crystals are badly needed.

We also note that, if the surface dangling bonds of Si grains are passivated by H atoms and if they are present in interstellar space in quantities sufficient to account for the observed ERE, we would expect to see the Si-H 15.6 \( \mu m \) wagging, 11.6 \( \mu m \) bending, and even 5 \( \mu m \) stretching bands (Adachi 1999).

Our analysis of NGC 2023 required the value of the foreground extinction \( A_{\lambda} \) to “deredden” the ERE measurements. Unfortunately, \( A_{\lambda} \) has not been directly measured at the location where the ERE observations were made. It would be extremely valuable to have ERE measurements made at a position where a reliable extinction has been determined—such as the emission bar 80' south of HD 39037—or to have both IR and far-red observations of \( H_2 \) emission (allowing \( A_{\lambda} \) to be determined) at a location where the ERE has been measured.

Our modeling has assumed isolated “free-flying” SNPs; we have demonstrated that existing DIRBE photometry for the diffuse ISM rules out the hypothesis that the observed ERE is due to such particles. Since isolated SNPs are ruled out, it is important to note that in the laboratory, photoluminescence is observed for SNPs located on a substrate (Ledoux et al. 2000). An SNP located on the surface of a large interstellar grain would have its temperature—and therefore its infrared emission—determined by the temperature of the “host” grain. In the case of NGC 2023, the radiation field is so intense that the “host” temperature would probably be similar to the temperature of the Si/SiO\(_2\) SNPs, so the 20 \( \mu m \) SiO\(_2\) emission feature should still be prominent, though its strength could be increased or decreased, depending on the optical properties of the “host” grain. In the diffuse ISM, the 20 \( \mu m \) emission feature would be completely suppressed if the SNPs are attached to larger host grains, with temperatures \( T \approx 15–20 \) K. Thus, SNPs attached to larger host grains may be a viable explanation for the observed ERE.

![Fig. 8.—Model IR emission spectra calculated for spherical grains (thin solid line), 5:1 prolate grains (dotted line), 5:1 oblate grains (short-dashed line), and grains with a distribution of spheroidal shapes (long-dashed line) illuminated by the NGC 2023 radiation field. All grains are taken to (1) be neutral, (2) have an equivalent sphere-volume Si core size \( a_{\mathrm{Si}} = 17.5 \) Å, and (3) have the Si core contributing 51% of the total grain volume. Also plotted are the ISO SWS spectrum (heavy solid line; Verstraete et al. 2001) and the KAO photometry (stars; Harvey et al. 1980). It is evident that our conclusions are insensitive to the assumed grain shape.](image-url)
The photoexcitation rate $\gamma$ for SNPs on the surfaces of $a \gtrsim 100$ Å grains would probably be lower than for free-flying SNPs, which would in turn increase the abundance of Si in SNPs required to explain the observed ERE. Since 42% or more of (Si/H)$_0$ is required even for free-flying SNPs with $\eta_{PL} f_0 = 1$, the Si abundance demands would be difficult to accommodate if the SNPs are attached to $a \gtrsim 100$ Å grains.

5. Conclusions

Table 2 summarizes our results for the abundances of Si/SiO$_2$ SNPs: upper limits based on nondetection of the 20 μm feature and lower limits (since $\eta_{PL} f_0 < 1$) if neutral SNPs are to account for the observed ERE, as argued by Smith & Witt (2001).

For Si/SiO$_2$ nanoparticles to explain the ERE observed in NGC 2023, nondetection of the 20 μm feature requires a luminescence efficiency $\eta_{PL} \geq 0.08 f_0^{-1} \times 10^{-4.4-6.8 \mu m}$, where $f_0$ is the fraction of SNPs that are neutral. Thus, for $A_{0.68 \mu m} = 1.2$ mag, Si/SiO$_2$ SNPs could account for the observed ERE in NGC 2023 provided $\eta_{PL} \geq 0.24 f_0^{-1}$. Photoluminescence efficiencies as high as 50% have been reported for Si/SiO$_2$ nanoparticles (Wilson, Szajowski, & de Filippo, 2001), and in principle $\eta_{PL}$ could approach 100%. However, if $A_{0.68 \mu m} \gtrsim 2.8$ mag, the ERE could not be due to Si/SiO$_2$ nanoparticles even if $f_0 = 1$, since the required $\eta_{PL}$ would then exceed 100%. A preliminary estimate of the SNP neutral fraction $f_0$ in NGC 2023 suggests that only a very small fraction $f_0 \leq 0.1$ of SNPs would be neutral. If so, it would be difficult to reconcile the observed ERE with a model where the luminescence is due only to neutral SNPs (even for $A_{0.68 \mu m} = 1.2$ mag one requires $f_0 \gtrsim 0.25$). We urgently need further study of SNP charging in NGC 2023 and other reflection nebulae with ERE, to obtain more reliable estimates of the neutral fraction $f_0$.

The ERE emissivity of the diffuse ISM (Gordon et al. 1998; Szomoru & Guhathakurta 1998) requires $\gtrsim 42\%$ (Si/H)$_0$ in neutral Si/SiO$_2$ SNPs, even for photoluminescence efficiency $\eta_{PL} \rightarrow 100\%$. Such a high abundance of SNPs in the diffuse ISM is difficult to reconcile with the evidence that a substantial fraction of interstellar Si is already locked up in amorphous silicate grains (e.g., see Weingartner & Draine 2001b). This difficulty is exacerbated if interstellar abundances are significantly subsolar, as has been argued (see Snow & Witt 1996; but see also Sofia & Meyer 2001, who argue that interstellar abundances are approximately solar).

We have calculated the IR emission that Si/SiO$_2$ SNPs would produce if they are free-flying. Existing DIRBE 25 μm photometry appears to already rule out such high abundances of SNPs in the diffuse ISM. If SNPs are responsible for the ERE from the diffuse ISM, we conclude that they must either be in $a \gtrsim 50$ Å clusters or attached to larger “host” grains. Future observations by SIRTF will be even more sensitive to the abundance of free-flying SNPs in the diffuse interstellar medium.

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### Table 2

| Region           | Composition | Si/H (ppm) from Observed IR Emission | Si/H (ppm) from Observed ERE Intensity$^a$ |
|------------------|-------------|------------------------------------|------------------------------------------|
| NGC 2023         | Si/SiO$_2$  | $<0.2$                             | $0.016 \eta_{PL} f_0^{-1} \times 10^{-6.4-6.8 \mu m}$ |
| Diffuse ISM      | Si/SiO$_2$  | $<2$                               | $15 \eta_{PL} f_0^{-1}$                  |

$^a$ The term $\eta_{PL} < 1$ is the photoluminescence efficiency for neutral SNPs, and $f_0$ is the fraction of SNPs that are neutral. Lower limits are obtained by setting $\eta_{PL} f_0 = 1$. The term $A_{0.68 \mu m}$ is the foreground extinction 60° south of HD 37903 at μm (see text).
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