Accuray of Stellar Opacities and the Solar Abundance Problem

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Abstract. The abundances of some of the most common elements in the Sun has been called into question by recent analysis based on new non-LTE hydrodynamic models. The new abundances of C, N, O, Ne etc. are 30-40% lower than the 'standard' solar abundances, which were heretofore well established and supported by precise helioseismological observations. A number of recent studies have addressed the issue from different perspectives. Given the inverse relation between opacities and abundances, another possible solution has been suggested: Upward revision of stellar opacities by about 10%. But the recalculation of astrophysical opacities by The Opacity Project (OP) and the OPAL groups has led to remarkable convergence in the final results, in spite of some fundamental differences in atomic physics and plasma physics. Deviations beyond a few percent level in the Rosseland mean opacities have been ruled out. However, we discuss the accuracy of the input physics in opacities calculations, as well as detailed monochromatic (as opposed to mean) opacities, that do in fact yield large differences in radiative accelerations derived from OP and OPAL data. In addition, we note sources of "missing opacity" that might bear on the solar abundances issue.

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INTRODUCTION

About 25 years ago two major projects — the Opacity Project (hereafter OP [1, 2]) and OPAL ([3], and references therein) — were initiated to recalculate in their entirety the then available astrophysical opacities. The efforts were launched in response to a "plea for re-examination" [4] of the older Los Alamos opacites, that failed to account for basic astrophysical phenomena such as the Cepheid pulsation period ratios when incorporated in stellar interior models. As is now well known, both OP and OPAL resulted in considerably higher opacities, by factors of 2-3 or higher, and did indeed solve the Cepheid pulsation problem and found many other astrophysical applications. Both projects involved an enormous effort, but employed quite different physical formulations for opacities calculations, for the atomic physics methods to compute the basic atomic data and the equations-of-state (EOS). Nevertheless, the final OP and OPAL results converged for the crucial quantity of interest, the Rosseland Mean Opacity (RMO), to within 10%.

However, in recent years several lines of investigation have revealed problems in stellar astrophysics related to opacities. The foremost is the unexpectedly large discrepancy in solar surface abundances, long regarded as the 'standard', and accurately determined from spectroscopy. But recently derived abundances from elaborate 3-D Non-Local-Thermodynamic-Equilibrium (NLTE) convection models imply a reduction in the most abundant light metals (CNONe) by an astounding 30-45% [5]. This discrepancy and possible causes have been amply discussed in literature The new reduced abundances are in serious conflict with those derived from accurate observations from helioseismology and stellar interior models. Aspects of this outstanding problem, and possible solutions, are addressed by a number of researchers; e.g. constraints on heavy-element abundances from stellar interiors ([6, 7]; an extensive discussion has recently been given by Basu and Antia [8], and references therein).

Stellar opacity is the common feature in stellar models. More to the point, the *absolute* accuracy of opacities directly determines the uncertainties in the models. The inverse relationship between opacities and abundances is obvious (To wit: Any increase in opacities would lead to commensurately lower abundances). It is estimated that an increase between 11-21% around the base of the solar convection zone $R_{\odot}(CZ) = 0.73R_{\odot}$ (Log T $\approx$ 6.34) may greatly ameloriate the situation. $R_{\odot}(CZ)$ is the boundary between the radiative and the convection zone, and is one of the tightly constrained parameters from helioseismology. Analyzing many stellar models, Basu and Antia ([8]) note that at least an increase of 10% is required (also John Bahcall, private communication). Thus we face the conundrum: The required increase is more than the level of agreement between OP and OPAL, but numerically not by a large amount compared to the enhancement already achieved. The logical conclusion is that higher precision is needed.

Stellar models also depend on the EOS and the exact temperature-density regime(s) where different elements and ionziation stages contribute. Bearing on the solar abundances issue, the chemical composition and the equation-of-state (EOS) of the Sun as inferred from seismic models, Trampedach *et al.* [9] have made a “synoptic" comparison of the EOS formalisms employed in OP and OPAL. The overall agreeement in the mean opacities conceals some major differences (see next section). Whereas the OP and OPAL RMOs agree reasonably well, Delahaye and Pinsonneault [6] find large differences of up to 80% for *radiative accelerations* g_{rad} for several elements from C to Fe. The g_{rad} are highly sensitive to the details of the monochromatic opacity, and other factors responsible for opacities computations such as the frequency resolution. Constrained by helioseismology, the EOS and the interiors models not only affect surface abundances but also ascertain fundamental parameters such as $R_{\odot}(CZ)$, the sound speed, and the helium abundance in the Sun. The level of precision and constraints does not accomodate the aforementioned large differences in solar parameters, which ought to be well established.

Advances in theoretical methods in the intervening two decades since the OP now enable much more accurate and consistent atomic data to be computed. A number of these developments were carried out by the OSU group, partially under the follow-up project to the OP called the Iron Project (Hummer *et al.* 1993; www.astronomy.ohio-state.edu/$\sim$pradhan). At the same time, the availability of high-performance massively parallel computational platforms also makes it possible now to undertake more accurate recalculation of opacities.

THE NEED FOR RE-EXAMINATION OF OPACITIES

This critical discussion entails the atomic physics of missing opacity, accuracy, and consistency of OP data. In the OP work about two decades ago we devoted considerable effort to compute atomic data using the state-of-the-art R-matrix method [2]. A primary feature of the R-matrix method is the inclusion of radiative excitations via autoionizing resonances in photoionization cross sections. But its application to large-scale calculations necessitated compromises in accuracy, as described in the seminal paper summarising the OP work (SYMP94 [1]). Some of these were: neglect of relativistic fine structure, high-energy cross sections, and inner-shell excitations.

In addition to accuracy, a bigger problem turned out to be completeness. The R-matrix calculations (even the non-relativistic version employed in the OP) became too cumbersome for the codes and computational resources available at that time. Therefore, a considerable amount of radiative data was computed with a much simpler atomic structure code called SUPERSTRUCTURE, or variants thereof. For example, most of the data for iron ions Fe VIII–XIII was thus obtained (referred to as the PLUS data in [1]). Based on OPAL work, it was known that these Fe ions are of crucial importance around the so-called Z-bump, vital for Cepheid pulsation models around Log (T) $\approx$ 5.2–5.3. That is because there are a huge number of M-shell transitions $n = 3 \longrightarrow n' \geq 3$. The problem with the inner-shell data was also redressed in the past few years [10].

Could there still be some atomic data that might result in missing opacity? In spite of the inclusion of inner-shell data, the outer-shell atomic data in the revised OP calculations remained the same (SYMP94). Therefore, a number of resonance complexes corresponding to several Rydberg series of levels were not included. Many calculations since the OP work, particularly under the Iron Project by OSU group, have shown that outer-shell radiative excitations into autoionizing resonances that lie *below* the inner-shell ionization energies are excluded. Fig. 1 compares photoionization cross sections of an excited state of two ions in the Boron isolelectronic sequence, O IV and Fe XXI, from OP and from more recent work. The cross sections exhibit huge *photoexcitation-of-core* (PEC) resonances (first identified by Yu and Seaton [1]). These complexes of (PEC) resonances converge on to the inner-shell ionization threshold energy with a large jump. But the crucial fact is that the effective cross sections are much higher than the OP data, and enhanced throughout the $n = 2 - 3$ energy range by up to two orders of magnitude.

As inferred from Fig. 1, the missing opacity may lie in an energy range from few eV to few hundreds of eV, depending on the element and ionization stage. Low-lying excited states of most ionization stages of abundant elements exhibit similar structures. This could be of direct relevance at temperatures and densities up to $R_{\odot}(CZ)$ around Log $T \sim 6$.

Apart from limited treatment of atomic structure, affecting accuracy and resulting in missing resonances, the OP atomic calculations were non-relativistic and in LS coupling. Therefore, a siginificant omission is that of intercombination transitions that involve spin-change but are permitted by change in parity and angular momentum. Although the total line strength in intercombination lines is only a fraction of that in dipole allowed transitions (no spin-change), both are E1 transitions and the effect is of the order of 15–20%. A limited number of intercombination lines ($n \leq 6$) were included later [10]. But, as mentioned above, since most of the OP data for Fe ions does *not* employ the R-matrix method, we expect the *absolute accuracy* to be no better than the OPAL data also computed using an atomic structure code (with a parametrized atomic potential). Therefore it would not be surprising if it is ascertained that there are systematic uncerainties in both the OP and OPAL data.

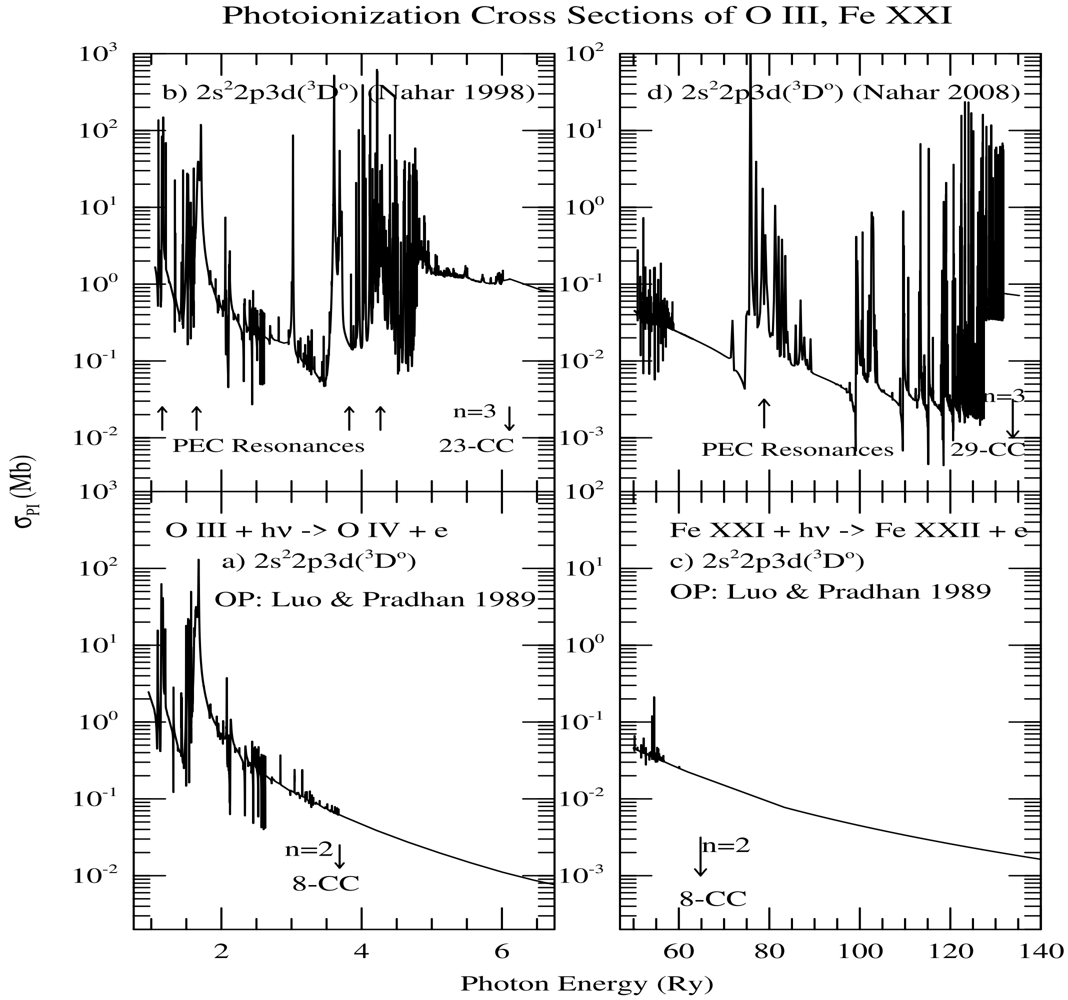

FIGURE 1. Missing resonances in photoionization cross sections of C-like O and Fe (e.g. Nahar 2008 [11]): bottom panels (a,c) — OP data, top panels (b,d) — more recent calculations which show that large resonance complexes were not included in OP data, and could account for some missing opacity. Note the abscissa in Rydbergs: 1 Ry = 13.6 eV.

Although much of fine structure splitting is subsumed by line broadening, a proper treatment should incoroporate relativistic fine structure more accurately than the current OP data. In the past few years, members of the OSU group, especially former graduate student G.X. Chen in collaboration with W. Eissner, have developed an extended version of the relativistic R-matrix method in the Breit-Pauli approximation used in the Iron Project work [12]. The OP data were computed or obtained in a variety of approximations and sources. In particular, the iron data was from six different sources, which raises some concern about consistency if not accuracy. And it was known that the loss of accuracy owing to restricted approximations for the low-ionization stages of iron Fe I–V, and other Fe-group elements, was especially severe [1, 10]. It therefore became necessary to include the corresponding transition probabilities from other sources. Although low ionization stages do not affect the RMOs in a signficant manner, they are crucial in computing radiative accelerations, and may well account for some of the large differences between OP and OPAL [6].

Equation-of-State

Dimtri Mihalas played the key role in the formulation of OP EOS. Together with David Hummer and Werner Däppen, Mihalas formulated the MHD-EOS[1] that was interfaced with OP atomic data on the one hand, and the opacities codes on the other hand (Hummer and Mihalas [15], Mihalas *et al.* [16], and Däppen *et al.* [17]).

The missing opacity may also arise from an EOS formulation with even marginally higher level populations in highly charged ions than the MHD-EOS. The general purpose of the EOS is two-fold: To determine thermodynamic properties involving derivatives with respect to temperature and pressure, and quantify parameters such as ionization fractions and level populations for opacities calculations. The initial OP calculations were for the *stellar envelope* region of stellar interiors (as defined in SYMP94), at temperatures and densiites outside the core: $T < 10^7$K and $\rho < 10^{-2}$ g/cc. That was primarily because the EOS adopted in the OP work, the MHD-EOS, was not valid in the deep interiors. The MHD-EOS is based on what is referred to as the “chemical picture", wherein atoms, ions, and nuclei are introduced a priori and perturbed by plasma interactions. The advantage of the MHD-EOS is that atomic properties and data can be computed for isolated atoms and ions. That is followed by implementing an occupaton probability (w_i) formalism to perturb atomic levels due to plasma effects and determine level populations. Thus the internal partition function for an atom(ion) of an element k in ionization state j is the weighted sum in the Boltzmann-Saha equation

$$U(i,j,k) = \sum_i w_i g_i exp(-E_i/kT), \tag{1}$$

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where E_i is the excitation energy of level i. Consistent with the restricted range of OP opacities, radiative atomic processes involving inner-shell were excluded from atomic data calculations. Both of these turned out to be significant sources of error and resulted in discrepancies with the OPAL opacities in the high-(T,ρ) regime. It also considerably limited the application of OP opacities to stellar models.

The EOS-atomic data problem was re-visited in the past few years by the OP The EOS-atomic data problem was re-visited in the past few years by the OP team [10]. The inclusion of inner-shell K and L shell excitations increased the OP opacities by up to $\sim$10% and brought about overall agreement with OPAL, with RMOs no different than a

[1] ‘MHD’ refers to the principal researchers: Mihalas, Hummer, and Däppen, and *not* the more common meaning “magneto-hydrodynamics".

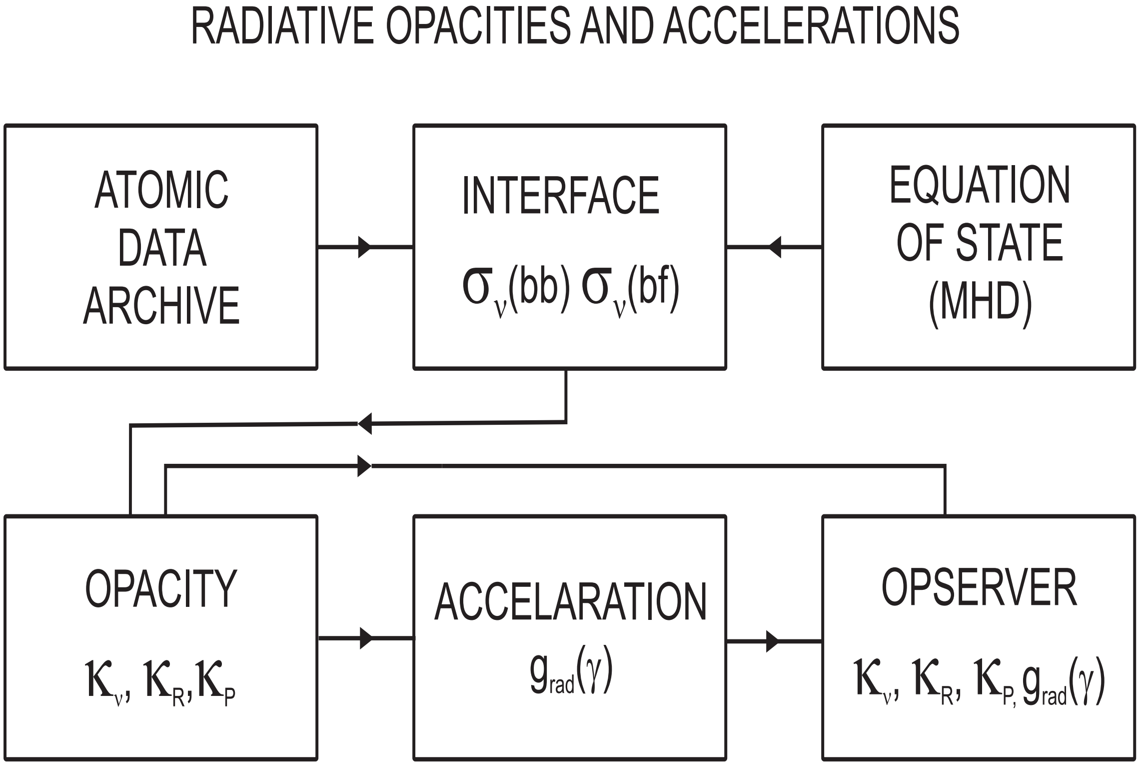

FIGURE 2. Schematic diagram of OP opacities computations.

few percent at most temperatures and densities. But in order to extend the MHD EOS to the deep interiors, an “expedient" was adopted by introducing an ad hoc critical cut-off value $w_c = 10^{-3}$ for the occupation probability. One consequence of this approach is to make the OP EOS much "harder" than the OPAL EOS, even by orders of magnitude in the numerical values of w_i. Clearly, the EOS issue also needs to be investigated (viz. Trampedach *et al.* [9]).

OPACITY AND RADIATIVE FORCES

Radiative forces and pressure may be computed in terms of the RMOs (M. J. Seaton [2] and references therein [18]). exerted by photons on a given atom may be readily computed, and photon absorption and scattering processes are responsible for radiation pressure. Opacities and radiative accelerations computed by OP have been made available from an electronic dataserver called OPSERVER (Mendoza *et al.* [13]), located at the Ohio Supercomputer Center at OSU and accessible from: *http://opacities.osc.edu*. Fig. 2 is a schematic diagram of OP opaciites.

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[2] This was Mike Seaton’s last paper. Seaton led the Opacity Project for over 25 years. He wrote most of the OP atomic physics codes, as well as another version of the opacities codes to verify the original version written by Yu, Mihalas, and Pradhan [1].

The OP atomic data is computed using the R-matrix codes or SUPERSTRUCTURE (or its variants). It consists of bound-bound (bb) transition probilities, bound-free (bf) photoionization cross sections, and other parameters such as electron impact damping constants. It is a non-trivial task to process all of the archived atomic data for proper input into the opacities code. It involves interface and mapping of data at computing energies on to a photon-frequency mesh. The standard variable for mapping is $u = h\nu/kT$. We define a "Rosseland window" in the range $-2.5 \leq Log\ u \leq 1.5$, which samples the monochromatic opacity with a given number of mesh points. Given the frequency-temperature correlation from the EOS, and the Planck function, the u-range is chosen so as to ensure that there is negligible contribution to opacity for any ion from outside the Rosseland window. These tasks are performed by the code INTERFACE, which also computes radiative line damping paramters using the bb-data (f-values for all allowed and intercombination E1 transitions). INTERFACE produces the bb and bf files for each ion.

The MHD EOS code independently produces tables of ionization fractions, scattering contributions, Stark broadening, and other parameters. The first calculation would be to use the standard EOS data as in the current OP. Later steps would follow as mentioned above.

The opacities code OPACITY requires the bb and bf atomic data files from INTERFACE, and the EOS tables. Calculations for the monochromatic opacity κ_ν are carried out for each ion along isotherms in Log T for a range of Log electron densities N_e. It is also useful to tabulate results along the variable R = ρ/T_6^3 ($T_6 = T \times 10^{-6}$) defined by OPAL. The Rosseland Mean Opacity κ_R is defined in terms of κ_ν as

$$\frac{1}{\kappa_R} = \frac{\int_0^\infty g(u)\frac{1}{\kappa_\nu}du}{\int_0^\infty g(u)du}, \quad g(u) = u^4 e^{-u}(1-e^{-u})^{-2}, \tag{2}$$

where $g(u)$ is the Planck weighting function (corrected for stimulated emission). The κ_ν is primarily a function of the oscillator strengths f, photoionization cross sections σ_ν, level populations N_i, and the line profile factor ϕ_ν,

$$\kappa_\nu^{bb}(i \rightarrow j) = \left(\frac{\pi e^2}{m_e c}\right) N_i f_{ij} \phi_\nu, \quad \kappa_\nu^{bf} = N_i \sigma_\nu. \tag{3}$$

Fig. 3 illustrates κ_ν(Fe IV) recently computed using the more accurate and extensive radiative R-matrix calculations by Nahar and Pradhan [14] including fine structure, compared to the original OP data. The difference in the Rosseland means is up to 50% at the (T, N_e) shown (close to maximum abundance of Fe IV). Although the Nahar and Pradhan calculations were also in LS coupling, they used a much larger wavefunction expansion (Eq. 2) than in the OP work. As noted, for such reasons the final OP calculations used the more complete bb data for lines of Fe I–V from the Kurucz database (which also includes fine structure). Fig. 3 shows the importance of completeness, but the accuracy issue is unresolved.

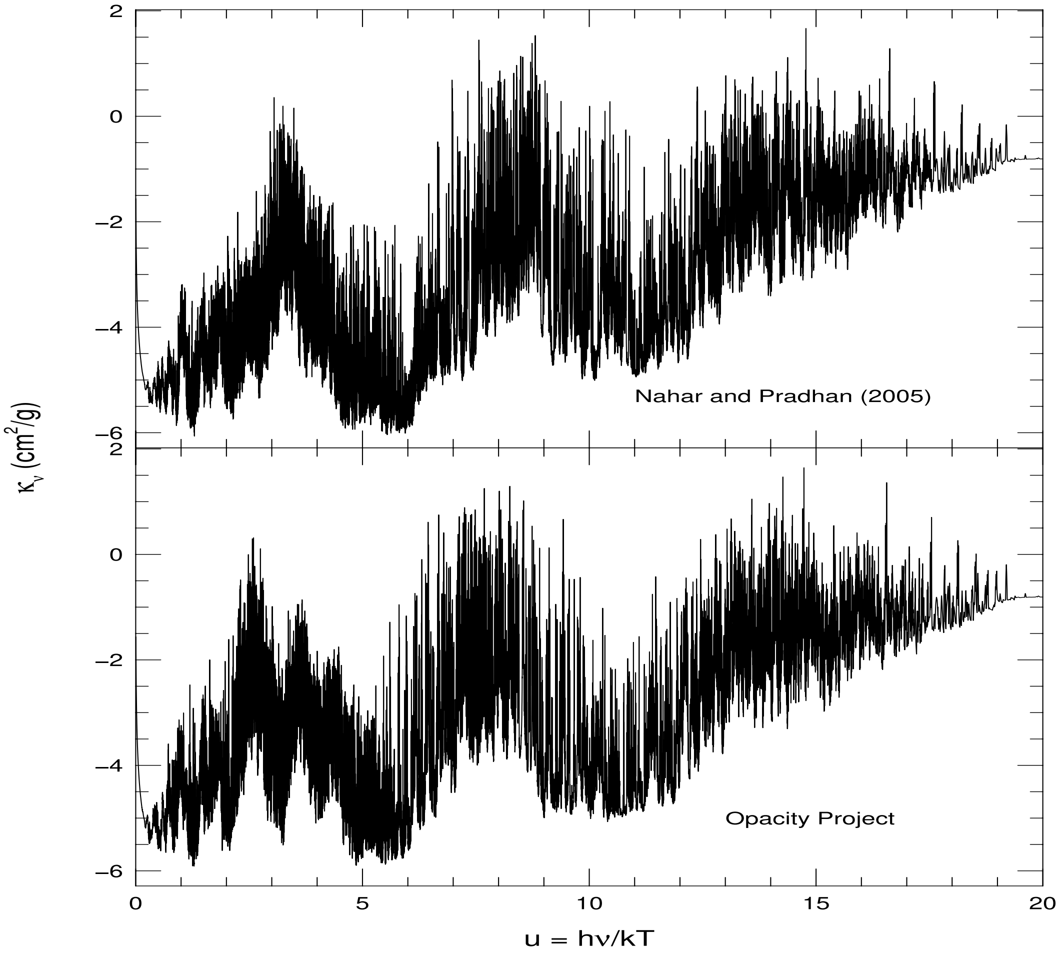

FIGURE 3. Monochromatic opacity of Fe IV at Log T(K) = 4.5 and Log $N_e(cm^{-3})$ = 17 — Recent calculations using new R-matrix calculations with fine structure (Nahar and Pradhan [14]), and the original OP data (SYMP94). Although the overall features look similar, there are considerable differences in detail and in Rosseland Mean Opacities of 10-50%.

SUMMARY

The possible solution to fundamental problems with solar models that have emerged in recent years may lie in stellar opacity. Helioseismology, equations-of-state, solar abundances, and stellar interiors models, are discordant in surprising and unexpected manner. The practical necessity of solving this problem can hardly be overstated, since the Sun is the key to understanding much of astrophysics. There is sufficient uncertainty in existing opacities calculations owing to the fact that resonances due to inner-shell excitations have not yet been fully included. Related effects such as autoionization widths, and plasma broadening, are not accounted for. As noted by stellar researchers, $\sim$10% revision of opacities would go a long way to resolving these discrepancies. At the same time, the minimum uncertainties in atomic physics are at least in that range, if not much higher. In addition, computed theoretical data reveal several sources of missing opacity or *systematic* inaccuracy in the approximations employed.

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