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RECENT PROGRESS ON ASTROPHYSICAL OPACITY

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Improvements in the calculation of the opacity of astrophysical plasmas has helped to resolve several long-standing puzzles in the modeling of variable stars. The most significant opacity enhancements over the Los Alamos Astrophysical Library (LAOL) are due to improvements in the equation of state and atomic physics. Comparison with experiment has corroborated the predicted large opacity increases due to transitions in M-shell iron. We give a summary of recent developments.

1. INTRODUCTION

Opacity plays an important role in astrophysical modeling affecting such things as the age of globular cluster stars, which are used to set a lower limit on the age of the universe; the luminosity function of Cepheid variables, which are used to set distance scales; and the density-temperature profile within the star, which determines the neutrino production rate and the seismic structure. Los Alamos National Laboratory has, since the mid 1960's, taken on the responsibility for providing the required data.

The inability to resolve a number of long standing discrepancies between theory and observation through improved modeling led to the speculation that the Los Alamos opacities were missing important sources of opacity in the 10^5-10^6 K temperature range[1]. Due to this speculation and the need for the opacity of low Z materials to model laser produced plasmas we initiated an entirely new an independent effort to calculate opacity in 1985. The equation of state and atomic physics bases of the Los Alamos Opacity Library[2] were the most likely sources that could lead to changes in the opacity. To improve the equation of state we use a many body expansion of the grand canonical partition function[3]; to improve the atomic data we use a parametric potential method[4]. The atomic structure calculations are done on-line and have accuracy similar to single configuration Hartree-Fock with relativistic corrections. A more detailed description of our approach, which we refer to as OPAL, is given in Ref. 5.

The first OPAL opacity tables were carried out using LS coupling to treat the configuration term structure and these results were widely distributed. Numerous improvements in theoretical agreement with observation were reported using the new opacities. For example, the mechanism for pulsation in β Cephei stars has been identified[6-8]; the "bump" and " beat mass discrepancies in Cepheid variables has been removed[9]; the period ratios for RR Lyrae stars agree closely with observation at evolutionary masses[9-11]; pulsation due to the epsilon effect is no longer predicted except for Pop I stars exceeding 120 solar masses[12]; the lithium depletion in the Hyades cluster stars and in the Sun is depleted compared to primordial values as observed[13]; the calculated solar seismic frequencies agree much better with observations[14-15]; and the brightness evolution of the star P Cygni now agrees with observation[16].

The success of the OPAL opacities in the resolution of these problems has encouraged us to introduce additional improvements in the calculations and to produce updated and expanded tables. The main physics improvement has been the inclusion of spin-orbit effects in the atomic physics calculations. Furthermore, in order to facilitate the calculation of large databases we have developed a corresponding states method. We have also studied the errors introduced by reducing the number of components in the mixture by combining the lesser abundant elements with prominent elements. A brief description of recent developments is given in the following sections.

2. ANGULAR MOMENTUM COUPLING

The Los Alamos opacity codes use a detailed configuration accounting method (DCA), that neglects term structure, to treat bound state absorption[17-19]. Introduction of term splitting in the LS coupling scheme was responsible for a major part of the enhanced opacity obtained by OPAL compared to LAOL in the few hundred thousand degree range[5,20,21]. The use of LS coupling is valid for low Z elements where the electrostatic energy dominates. The spin orbit interaction is very small for Z<10, but increases with increasing Z leading to lifting of the J degeneracy and to the appearance of intercombination lines. The coupling in this case is intermediate between pure LS and pure jj. For intermediate Z elements, such as iron, the spin orbit interaction produces small, but important effects. The different coupling approaches are illustrated in Fig. 1 for the case of transitions of the type sp to p^2. In the DCA approach there exists a single line. LS coupling-splits this line into three components corresponding to singlets and triplets. In intermediate coupling the spin orbit effect further splits the spectrum into 8 lines having $\Delta S = 0$ and 6 intercombination lines; 3 lines having $\Delta S = +1$, and 3 lines having $\Delta S = -1$. For more complicated configurations the increase in the number of distinct lines can be much larger.

The splitting into additional lines distributes the oscillator strength more uniformly over frequencies and is similar to increasing the line width. The introduction of intermediate coupling can, thus, further increase the opacity when the spin orbit "broadening" exceeds the line broadening. Since the spin orbit effect does not depend on density, while line broadening does, its effects become more important at low density. This is illustrated in Fig. 2(a-c), which compares the OPAL intermediate coupling result to the LS coupling result for several values of R vs. T_6, where $R=\rho/T_6^3$, $T_6=T/10^6$K, X is the hydrogen mass fraction, and in this context Z is the mass fraction of all elements heavier than helium. The intermediate coupling scheme gives an enhancement of 50% at Log R=-5 and T_6=0.25, whereas the enhancement is insignificant at log R=-2. A more complete description of this work is given in Ref. 21.

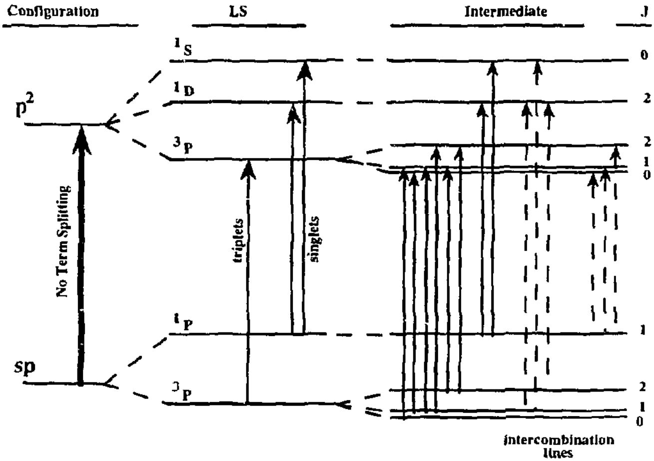

FIGURE 1
Schematic drawing showing various angular coupling schemes.

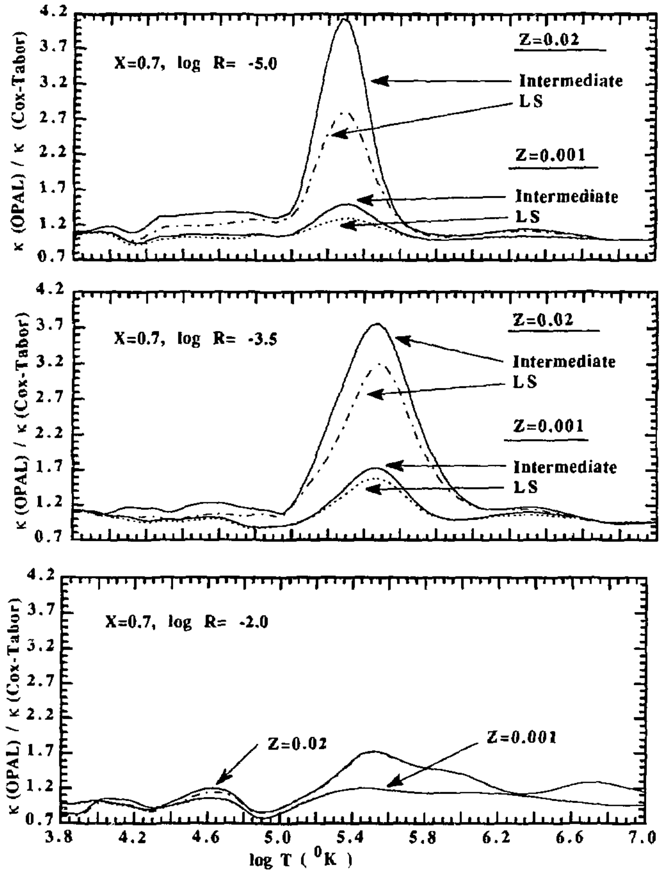

FIGURE 2
Intermediate coupling effects on the Rosseland mean opacity. OPAL results are shown normalized to Cox-Tabor[18] opacities.

3. VARIABLE MIXTURES

Stellar plasmas are composed of at least 99% hydrogen and helium by number fraction, except for advanced type stars which have burned these elements. At low densities, such as occur in stellar envelopes, the equation of state is dominated by ionization equilibrium of H and He. There are, nonetheless, corrections of order a few percent, due to Coulomb correlations. Corrections of about 1% arise due to the ionization equilibrium of elements having Z> 2. Even so, both of these terms are large enough to play an important role in the seismology of stars[15]. Under these conditions the ideal gas mixing of pure components works very well. This is the approach adopted by LANL to calculate their opacity library.

The pure element mixing approach is not valid at high density were the plasma is strongly coupled. Consequently, in our work we calculate the equation of state for the full mixture, including the Coulomb coupling between the various constituents. However, even in this case simplification is possible. It can be shown[22] that the intra-ionic ratios for ions of type i in the various states of ionization can be the same for mixtures having different elemental mass fractions, χ_i, and densities. The conditions for this to occur is that the temperature and electron number density be the same. It follows that a solution for the equation of state for a mixture characterized by T, n_e, ρ, and χ_i can be used to find the equation of state for a different mixture characterized by T, n_e ρ', and χ_i'. The electron density for the initial and final mixtures are given by

$$n_e = \rho \sum_i Q_i^* \chi_i / A_i \qquad \text{and} \qquad n_e = \rho' \sum_i Q_i^* \chi_i' / A_i \tag{1}$$

where Q_i^* is the average state of ionization for element i and A_i is the atomic weight. The densities of the two mixtures are thus related according to

$$\rho' = \rho \left\{ \sum_i Q_i^* \chi_i / A_i \right\} \left\{ \sum_i Q_i^* \chi_i' / A_i \right\}^{-1} \tag{2}$$

Since the relative intra-ionic occupation numbers are the same in the two mixtures, it is possible to rapidly calculate the opacity of the second mixture from the data already calculated and stored for the first mixture. We have used this approach to expand the tables in the hydrogen and metal mass fractions X and Z[22]. The current tables cover 10 values of X in the range 0 to 1-Z and 13 values of Z in the range 0 to 0.1.

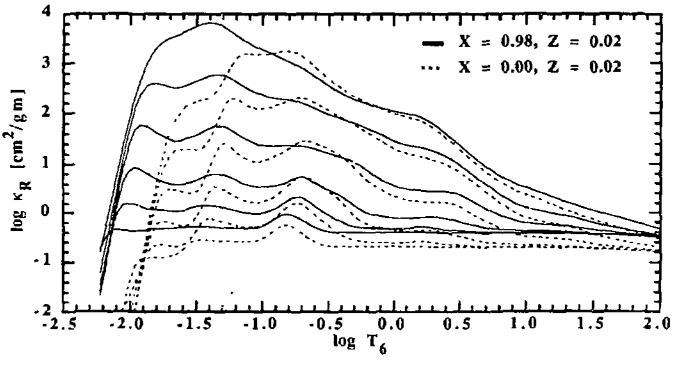

FIGURE 3
Comparison of κ_R for X=0 and 1-Z. The curves are for constant R values: (from top to bottom) log R= -1, -2, -3, -4, -5, and -7.

Fig. 3 shows log κ_R vs log T_6 for the extremes of X when Z=0.02. A number of differences related to the H abundance in the mixture are apparent. There is a rapid rise in opacity at low temperatures which is caused by the ionization of hydrogen when X=1-Z and to the ionization of helium when X=0. In the latter, the higher ionization potential of He shifts the onset of this rapid increase in κ_R towards higher temperatures. The opacity bump occurring near log T_6=-0.7 is more pronounced for X=0 and is due, in part, to the photoionization of the K-shell electron in singly ionized He. In addition, there are relatively more metals by number in the X=0 mixture further enhancing the bump near logT_6=5.2. Finally, the lower electron density of the X=0 composition leads to lower photon scattering and free-free absorption contributions; consequently, its opacity is lower at high temperatures.

Due to the versatility of the corresponding states method we can use the stored occupation number and photoabsorption data to rapidly calculate opacity tables covering the same range of X and Z for arbitrary heavy element abundances. We are currently producing tables for advanced type stars that have enriched He, C, and O abundances.

4. HEAVY ELEMENT ABUNDANCE EFFECTS

We have shown that uncertainties in heavy element abundance can produce opacity changes of the same size as the as the calculational uncertainty[21]. A recent 30% downward estimate in the spectrographically determined photospheric iron abundance reduced calculated opacities by about half the amount of the increase due to the spin orbit interaction (see Fig. 2).

An artificial adjustment in heavy element abundances is introduced in opacity calculations due to a need to reduce computer expense. Since some elements have very low abundance compared to their neighbors, it is common practice to lump the abundance of these elements with the more abundant neighbor. The opacity tables given in Ref. 5 were for H, He, and a twelve element composition for Z. In particular we added Cr and Ni together with Fe. Fig. 4 shows the ratio of the OPAL opacities vs temperature at log R=-5 for a 16 element mixture that treats Cr, Fe, and Ni as distinct components in contrast to the 14 element mixture in which Cr and Ni have been combined with the Fe. A substantial enhancement of about 28% occurs around T_6=0.25. Similar results have also been obtained by the opacity project[23]. Even so, this enhancement is small compared to the factor of 4 obtained over LAOL with the introduction of LS coupling.

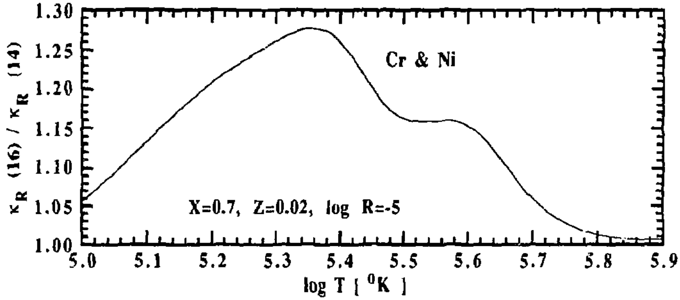

FIGURE 4
Effect of including Cr and Ni explicitly in mixture.

Fig. 5 gives the frequency dependent absorption cross section for Cr, Fe, and Ni at $T_6=0.2$ and log R=-5. Due to the Z^2 scaling of the energies, valleys in the Fe absorption are filled in by strong features in the Cr and Ni spectrum. In such cases, it is not a good approximation to treat the Cr and Ni as though their spectrum is the same as that of Fe. This was also *noted earlier*[5] , *where only the enhancement due to Ni was considered.* Revised tables including Cr and Ni are being calculated.

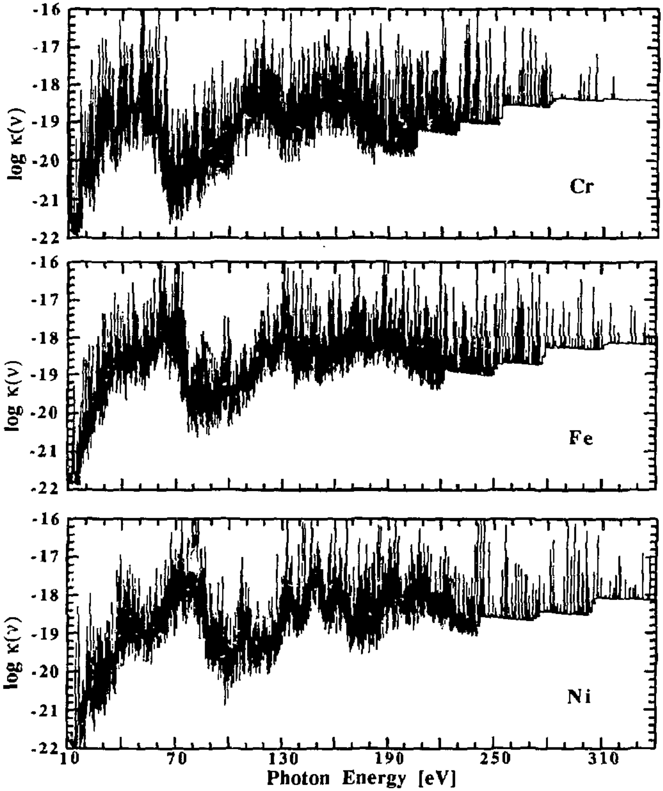

FIGURE 5

Photoabsorption coefficients (cm^2/ *nuclei) for* Cr, Fe, *and* Ni *for a plasma at* logT=5.3 and logR=-5. Note similarity, but also small shift towards higher photon energy with increasing nuclear charge.

5. OPACITY EXPERIMENTS

Even though opacity plays a crucial role in stellar evolution and pulsation, reliable measurements have only recently started to become available. The temperature density range covered by stellar plasmas is very large and not accessible by a single method. So far, two types of experiments that access very different temperature and coupling ranges have been carried out. One accesses the hot (> 20eV) weak coupling region; the other the low temperature (< 1 eV) moderate to strong coupling range. The procedure used to obtain hot plasmas involves two laser beams, one to heat a thin metal sample up to several hundred thousand degrees and the other to act as a backlighter source. The measured transmission of the backlighter source, $\exp(-\rho L\kappa(\nu))$, where ρ is the sample density and L the sample thickness, yields $\kappa(\nu)$, the frequency dependent opacity [24]. The procedure to obtain relatively cold plasmas is based on gas gun technology and is described elsewhere this volume[25]. The gas gun method has the advantage that it also obtains the equation of state.

Compared to LAOL the OPAL calculations show differences in at least three important regions: 1) A 20% decrease in opacity in the 3×10^4-10^5 K temperature region, due to improved line broadening; 2) An increase of as much as a factor of 4 in the 10^5- 10^6 K range, due to improved atomic physics; 3) An increase of 10-20% in the few million degree range, due to improved equation of state. These differences with LAOL, as mentioned briefly in Sec. 1, have each made significant improvements in stellar modeling. The predicted large enhancements to astrophysical opacities due to transitions in the M-shell of iron; particularly the $\Delta n=0$ lines around 70 eV, are the most interesting from an experimental point of view . This M-shell structure has a strong affect on the Rosseland mean in the 20 eV temperature range. So far two experiments have been completed that test the validity of the OPAL code for treating absorption in hot iron plasmas. The first[26] studied pure Fe at $\log T\approx5.4$ and $\rho\approx0.008$ g/cm^3 and was design to observe the prominent $\Delta n=0$ features. Since the calculations predict that these features persist over a wide range of temperature and density, the diagnostics in the experiment were not designed to make accurate measurements of plasma conditions. As a result, the temperature uncertainty is 20% and the density is estimated to within a factor of two.

The results of the Da Silva *et. al.* experiment are compared with two versions of OPAL in Fig. 6. It is apparent that DCA calculations with hydrogenic oscillator strengths, which closely approximates the LAOL calculations, has no absorption features in the crucial 70 eV photon energy range; whereas both the OPAL calculation with full intermediate coupling and the experiment show strong absorption features in this range. The experiment thus offers confirmation that the OPAL prediction is qualitatively correct.

The second experiment[27] introduces a small impurity of NaF in the Fe sample in order to determine the plasma temperature using an established method [24]. They also developed a technique to determine the density accurately. The purpose of this experiment was to measure the frequency dependent absorption over the energy range that contributes most to the Rosseland mean in a well characterized experiment; the first such experiment in a hot plasma. The conditions were determined to be $kT=59\pm3$ eV and $\rho=0.0135\pm0.0014$ g/cm^3. Integration over the experimentally obtained k(n) gave $\kappa_R=4400\pm600$ cm^2/g. The OPAL result for nominal conditions is 4100 cm^2/g. This experiment, thus, also supports the OPAL results.

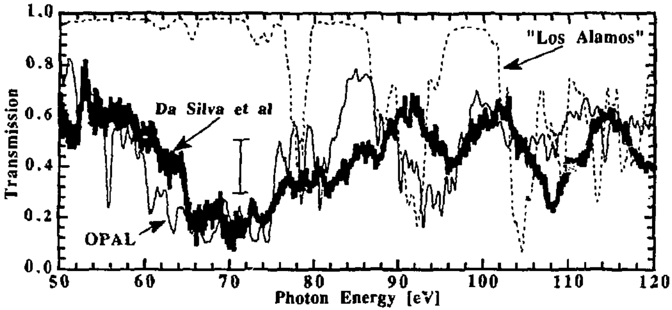

FIGURE 6
The Fe transmission experiment (heavy solid line) is compared to OPAL with intermediate coupling (thin solid line) and OPAL in DCA with hydrogenic oscillator strengths (dashed line) simulating the LAOL calculations. Experimental error bars for the transmission are indicated in the figure.

6. Conclusion

Refined stellar modeling is dependent on good input physics. The protracted attempts to determine the mechanism for β Cephei pulsation and to remove the Cepheid mass anomaly demonstrates the futility of fine tuning models that are based on poor input physics. The large number of calculational properties improved solely through use of improved opacities shows clearly the value of such efforts.

Recent laser experiments on thin metal foils have corroborated the large $\Delta n=0$ contribution from M-shell iron predicted by OPAL and verified the Rosseland mean at one temperature density point. This is strong evidence that the OPAL opacities represent a significant improvement over LAOL. The close agreement[23,28-29] of OP and OPAL (Pradhan this volume) in the range where OP is valid (ρ <0.01 g/cm^3) is additional strong evidence, supporting both efforts.

We have continued to improve and update the OPAL opacity calculations. Substantial increases in opacity over our earlier work were obtained with the introduction of intermediate coupling; particularly at low density where the spin orbit splitting can be greater than the spectral line broadening. Significant increases in opacity were also obtained by explicitly including the lowly abundant Cr and Ni in the metal mixture; clearly showing that even elements of very low abundance can make important contributions when their spectrum fills in valleys where no other element has absorption features. This again demonstrates that accurate opacities also require an accurate determination of the stellar element composition.

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