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RESULTS OBTAINED USING THE OPAL CODE

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RESUMEN. Las opacidades medias de Rosseland calculadas con el programa OPAL se comparan con los resultados de Los Alamos, encontrando diferencias de factores de tres. Estas diferencias se atribuyen a los adelantos, tanto en la ecuación de estado como en la física atómica, del programa OPAL. Más aún, investigaciones recientes han demostrado que las nuevas opacidades de OPAL eliminan las discrepancias entre las observaciones y los modelos estelares.

ABSTRACT. The Rosseland mean opacities computed using the OPAL codes show significant differences when compared to the Los Alamos results. The differences have been traced to improvements in both the equation of state and atomic physics in the OPAL code. Furthermore, recent work suggests that the OPAL opacities considerably improve the agreement between observations and stellar models.

Key words: OPACITIES – SUN: INTERIOR – STARS: VARIABLE

I. INTRODUCTION

The transport of energy in the interior of stars is primarily through photon radiation, convection, and electron conduction. Of the three processes, radiative transport is perhaps the most essential in governing the structure and evolution of a star. However, there are no direct measurements of the radiative opacity at stellar interior conditions so that one must rely on theoretical calculations. At present, there are promising efforts to correct the situation (Davidson et al 1988). Fortunately, there are observable stellar properties which are sensitive to the opacity. Therefore, comparisons of stellar models and observations provide an indirect test of the theoretical opacity. In fact, the comparisons suggest that the Los Alamos opacities, which for more than two decades have served as the standard, are in error. For example, several researchers have shown that large opacity enhancements at $T \approx 300{,}000$ K can resolve mass anomalies between evolution and pulsation theories (Stellingwerf 1978; Simon 1982; Andreasen and Petersen 1988; Andreasen 1988; Petersen 1989,1990). Inspired by his result, Simon suggested that the opacity may indeed be underestimated for temperatures above 100,000 K and speculated that the deficiency was due to approximations in the calculation of photon absorption processes of heavy elements.

Magee, Merts, and Huebner (1984) responded to Simon's plea for a re-examination of the metal opacity and concluded that such large opacity increases were incompatible with atomic physics. Contrary to their claims, Simon's speculation has been subsequently substantiated by the OPAL code (Iglesias, Rogers, and Wilson 1987, 1990; Iglesias and Rogers 1991b; Rogers and Iglesias 1992) with the opacity enhancement attributed to improved atomic physics. Independently, Rozsnyai (1989) has bracketed the opacities using an approximate treatment to account for the large number of spectral lines and obtained minima and maxima compatible with Simon's speculation.

A number of other studies demonstrate sensitivity to opacity. Several groups have considered the p-mode eigenfrequencies in the Sun (Christensen-Dalsgaard et al. 1985; Korzennik and Ulrich 1989; Cox et al. 1989, 1990) and all concluded that increases in the Los Alamos opacities of approximately 20% near the bottom of the convection zone brings models and observations into better agreement. Again, such an increase in opacity has been substantiated (Iglesias and Rogers 1991a). The lithium depletion problem in the Hyades cluster has been addressed by Swenson, Stringfellow, and Faulkner (1990) who showed that increasing the Cox-Tabor (1976) opacities by 37% near $T=4x10^6$ K reduces the computed lithium abundances to values consistent with observational constraints.

Finally, not all attempts to resolve the discrepancies between models and observations depend on opacity changes. For example, Carson and Stothers (1988) suggest a luminosity increase to bring into virtually perfect agreement pulsation models with observed ridge-like classical bump Cepheids. Nevertheless, the existing discrepancies are sensitive to the opacity and they will be difficult to eliminate until uncertainties in opacity calculations are better understood and substantially reduced. As a result, at least two major independent efforts are underway to recompute opacity tables. One is the Opacity Project (see this Volume). The other is our own, which we refer to as OPAL. Two OPAL tables have already been published but these are somewhat specialized. The first is for the solar radiative interior (Iglesias and Rogers 1991a) and the second is for Cepheid variables (Iglesias and Rogers 1991b). More extensive OPAL results which allow accurate interpolation in temperature, density, hydrogen mass fraction, and metal mass fraction are now available (Rogers and Iglesias 1992).

II. THE OPAL CODE

The OPAL code removes several approximations in the equation of state (EOS) and atomic data generation present in past calculations. Although there are EOS issues which can affect the opacity, the most significant opacity enhancements reported are due to improvements in the atomic physics. The OPAL code is described in detail elsewhere (Rogers and Iglesias 1992). Briefly, it uses the method of detailed configuration accounting; that is, it considers ion stages and their electron configurations (including term structure) explicitly from the start. The EOS and occupation number calculations are based on a renormalized activity expansion for the pressure in the grand canonical ensemble as described by Rogers (1986). The method avoids the *ad hoc* cutoff procedures necessary in free-energy minimization schemes (e.g., Huebner et *al* 1977; Hummer and Mihalas 1988). Note that we do not follow the ideal gas mixing procedure described in Huebner et *al* (1977) for combining the various photon absorption coefficients from the different elements. Instead, coupled equations for the full mixture are solved at each density and temperature point.

The detailed configuration accounting approach requires atomic data which is computed using parametric potentials (Rogers, Wilson, and Iglesias 1988). The method yields atomic data (energy levels, oscillator strengths, and photoionization cross sections) comparable in accuracy to single-configuration, self-consistent field calculations with relativistic corrections. Consequently, it is much more accurate than the approximations used for generating atomic data in previous opacity tables (e.g., Weiss, Keady, and Magee 1990). It is important to note that our atomic calculations have a reasonable degree of accuracy not only for valence electrons but also for photon absorptions involving inner core electrons as well as multiply excited ions. Both of these processes are necessary in determining the Rosseland mean opacity. The OPAL code does include autoionizing lines, but treats them simply as ordinary lines. That is, it ignores the possible interference effects between the final bound state and the continuum which requires configuration interaction calculations (e.g., Seaton 1987).

The function of the parametric potentials is to provide radial wavefunctions and configuration-averaged energies. A second phase of the calculation requires the determination of the energy-level structure due to the Coulomb interaction between electrons plus spin-orbit terms. This is accomplished by applying standard perturbation theory (Cowan 1981). At present, the atomic data in OPAL neglects the spin-orbit interactions and assumes pure LS-coupling. Note, however, that uncertainties in the angular momentum coupling scheme have been investigated in Rogers and Iglesias (1992) where intermediate coupling results have been considered. Even though it is possible to treat all configurations in LS-coupling, it is very time consuming. More importantly, it is wasteful since highly excited electrons are well approximated by hydrogenic formulas. Below, we delineate the approximations to the angular momentum coupling currently in the OPAL code. We also discuss briefly the treatment of spectral line broadening, inverse bremsstrahlung, and photon scattering.

Photoionization processes are considered individually for every subshell in every electron configuration of the various ion stages. Calculation are done in the central field approximation for electrons with n greater than 4. For n less than 5, we include the configuration term splitting in the LS angular momentum coupling scheme. We also include the bound-free absorption from H^- (Wishart 1979), since it can dominate the absorption at low temperatures.

The bound-bound transitions are calculated for every subshell in each configuration of the various ion stages explicitly. The energies and oscillator strengths of absorption lines are computed in LS coupling for transition electrons with both initial and final n less than 5. For jumping electrons with initial n greater than 4, configuration term splitting is neglected and transitions are computed for the nl subshell only. For electrons with initial n less than 5 but final n greater than 4, the lower configuration term splitting is included in LS coupling. Transitions to states with $n > 10$ are not explicitly included, but instead are approximately treated by extending the photoionization cross sections to lower photon energies.

Three additional approximations are made with regards to the angular momentum coupling. Due to memory and computer time constraints the number of lines in a single configuration-to-configuration transition array is restricted to 10,000. At present, if the actual number of lines is greater, the term splitting is ignored and only a single, average line is considered. For similar reasons the term splitting is neglected for spectral lines with energies greater than 13.5 kT (kT=temperature in energy units). At these higher photon energies the Rosseland mean weighting function is less than 1% of the peak value and the details of the bound-bound transitions should not affect the Rosseland mean opacities. Finally, excited spectator electrons with n greater than 5 are included in the calculation of the configuration-averaged energies and wavefunctions, but are not included in the angular momentum coupling. This approximation reduces, in principle, the number of spectral lines in the calculation. However, these electrons reside in large orbits which do not couple strongly to the actual jumping electron. Furthermore, they usually belong to configurations of low abundance.

Except for some special cases, line shapes are assumed to be Voigt profiles with Doppler broadening and the Lorentz width given by electron impact formulas from Dimitrijevic and Konjevic (1980, 1986, 1987). Their electron impact formulas require radial dipole integrals which are obtained using the wavefunctions obtained from our parametric potentials. The exceptions are for the Lyman and Balmer series of hydrogenic systems for which we include fine structure and linear Stark effects due to ion electric microfields using subroutines generously provided by Lee (1988). Similar subroutines are used for the Lyman series of helium-like ions and transitions out of the $n = 2$ level in lithium like ions. For one-electron systems we have modified the method by Griem (1960) in order to treat transitions from levels with n greater than 2. The modifications involve improved ion microfield distributions (Iglesias et al. 1985) and electron impact widths (Lee 1988).

Although the line shape codes by Lee (1988) have been extensively checked against experiment and other codes, here we present a test of their implementation in OPAL. In Fig. 1, emission coefficients from OPAL are compared to the Balmer spectrum measured by Wiese, Kelleher, and Paquette (1972) in a high-current, wall-stabilized arc operated in hydrogen. In making the comparison it is important to remember that the experiment is probably not in thermal equilibrium (assumed in the OPAL calculation) and that the quoted temperature and electron density have experimental errors. Nevertheless, the OPAL result is in good agreement with the experiment which suggests that the line shape theory is realistic, at least in the near wing (the far wing is not tested since it is obscured by the H^- absorption).

Unfortunately, the Wiese et al. experiment is not a sensitive test for EOS or occupation numbers, but rather it is an excellent test for Stark broadening of hydrogen spectral lines as originally intended by Wiese et *al.* The reason is that a simple Saha-type EOS formulation with principal quantum number cut-off above the Inglis-Teller limit (Inglis and Teller, 1939) will reproduce reasonably well the experimental data (Dappen, Anderson, and Mihalas 1987). The difficulty is in reproducing the line spectra near threshold where a careful theory would need to Stark mix many states of different principal quantum numbers plus the continuum. Present line shape theories do not include this coupling and therefore have unphysical broadening to regions far from line center leaving a spectral window near threshold. To avoid this problem, we have incorporated a phenomenological method (D'yachkov, Kobzev, and Pankratov, 1988) that mimics the line broadening of overlapping lines. Other authors (see for example, Ruzdjak and Vujnovic 1976; Dappen et al. 1987; Seaton 1991) have used similar schemes with reasonable success. All of these schemes, however, are in effect smoothing procedures which conserve oscillator strength and restrict the line radiation to the region near threshold.

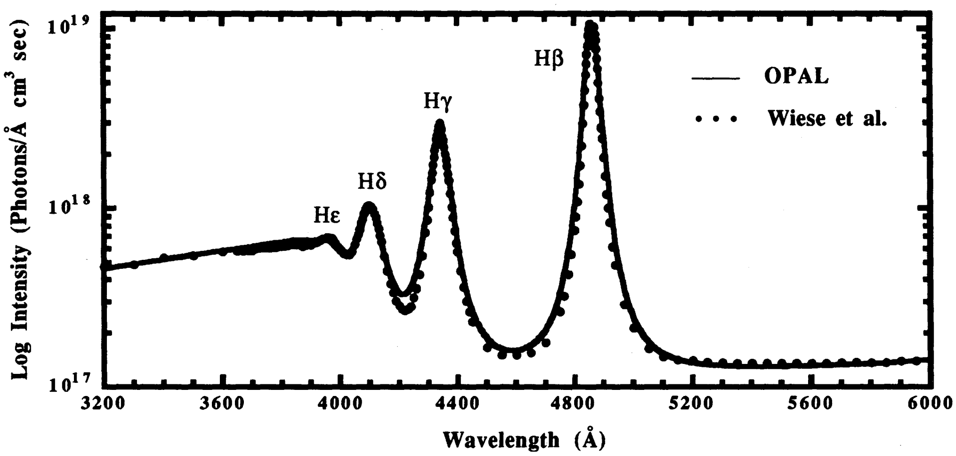

Figure 1 --- Comparison of OPAL and hydrogen emission experiments by Wiese, Kelleher, and Paquette (1972). The experimental conditions are T=13,000K and 9.3×10^{16} free electrons/cm^3.

Inverse bremsstrahlung is computed using the parametric potentials including plasma screening effects. Whenever possible approximate methods are used to evaluate the free-free gaunt factors. We use an elastic scattering approximation for small photon energies and the Born-Elwert approximation at large photon energies (Johnson 1967). Otherwise, the brute force calculation of the dipole matrix element is done. In all cases the required thermal averages are done with the Fermi-Dirac distribution for the electrons, including the Pauli exclusion principle for final states (Huebner 1986). We do not consider inverse bremsstrahlung for neutral atoms except for H (Stilley and Callaway 1970) and He (Somerville 1967). These calculations for the neutrals do not include plasma effects. However, if the absorption is dominated by the neutrals, then the charged particle density is relatively low, minimizing any screening effects.

The photon scattering from electrons is treated by a method described by Boercker (1987) modified to include relativistic corrections (Sampson 1959; Huebner 1986). In his approach, Boercker treats electron correlations through the ring approximation plus first order exchange terms. We also include Rayleigh scattering from neutral hydrogen and helium using the fits in Kurucz (1970).

III. ASTROPHYSICAL APPLICATIONS

As mentioned earlier, there are no direct measurements of opacities at stellar interior conditions. Therefore, it is important that theoretical results be applied in stellar models and the consequences tested against the available observational data. Below, we compare the OPAL opacities to the Los Alamos results and find significant differences. In addition, several studies that apply the OPAL opacities are briefly discussed. We emphasize the effects these differences in opacity have on astrophysical problems.

III.a *Solar Radiative Interior*

The solar neutrino flux and helioseismology are sensitive to the opacity of the solar radiative interior (e.g., Bahcall and Ulrich 1988). In an effort to reduce and understand the opacity uncertainties, we have computed tables for the solar interior (Iglesias and Rogers 1991a). The OPAL results for the Grevesse (1984) composition are compared to those from the Los Alamos Astrophysical Opacity Library (Huebner et *al* 1977) in Fig. 2. Our results are a few percent higher near the solar center (T_6~16), where T_6 is temperature in million of degrees) and about 10% higher near the bottom of the convection zone (T_6~2). The opacity enhancement near the bottom of the convection zone is welcomed by the helioseismology community (e.g., Christensen-Dalsgard, Gough, and Thompson 1991). On the other hand, the opacity enhancement makes the neutrino problem worse. However, the neutrino problem may be resolved with new physics requiring the predicted high SNU rate (Bahcall and Bethe 1990).

We note that, although the situation is improving, the solar element abundances are not known very accurately. OPAL results for solar compositions obtained from other observations are presented in Fig. 3 where now the OPAL calculations for the Grevesse (1984) mixture are used as reference. Figure 3 clearly shows that the opacity variations due to various solar compositions is comparable to code variations. It seems that even if very accurate opacity calculations were possible, the uncertainties in element abundances from observations would not remove all opacity errors in the solar models. Nevertheless, it is important to pinpoint the cause for disagreement between the codes. We have found (Iglesias and Rogers 1991a) that uncertainties in inverse bremsstrahlung, line broadening, and configuration term splitting are responsible for a few percent differences in the Rosseland mean opacity for solar interior conditions. Photon scattering from free electrons can lead to as much as ~10% errors at the solar center, but only if the crudest approach is used. The main source of uncertainty (~10%) is in the EOS result for the ion balance near the convection zone.

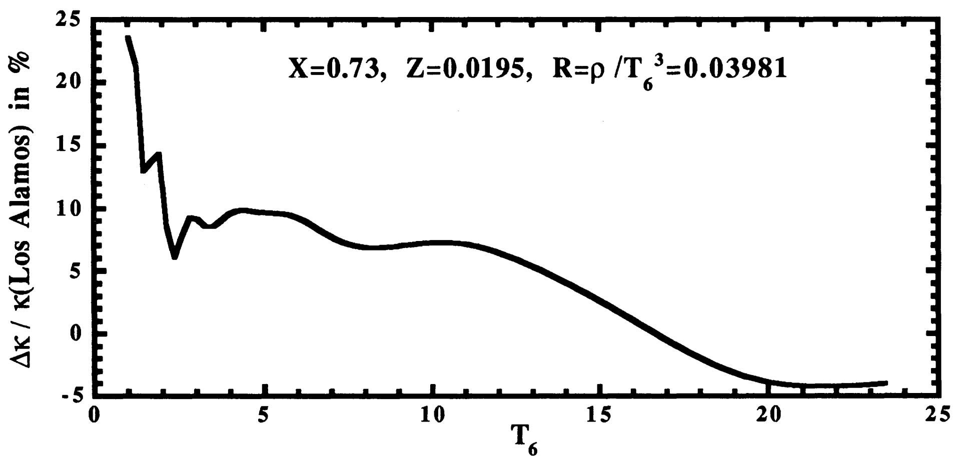

Figure 2 --- Comparison of OPAL to the Los Alamos Astrophysical Opacity Library (LAOL) for the Grevesse metal composition along a density-temperature track defined by constant ρ / T_6^3 where ρ is the density in gm/cm^3 and T_6 is the temperature in units of 10^6K. Here, X and Z are the hydrogen and metal mass fraction, respectively.

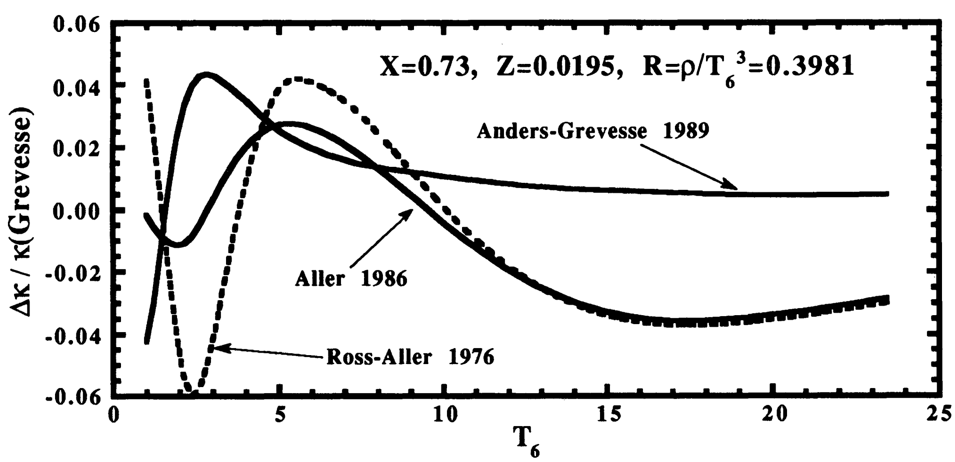

Figure 3 --- Comparison of OPAL opacities for different compositions for same conditions as in Figure 2. Here, OPAL results for the Grevesse (1984) composition are used as reference.

III.b *Variable Stars*

Among the outstanding unsolved problems in stellar evolution and pulsation theory is the modelling of multimode stars. As mentioned earlier, the opacity is a critical factor in determining stellar pulsation properties. Presented in Fig. 4 are the OPAL opacities and the Stellingwerf fits (Stellingwerf 1974, 1975) to the Cox and Tabor (1976) results for Population I and Population II compositions commonly used in stellar models. The R and Z values chosen for display are typical for Cepheid variables. The bump in the opacity near LogT=4.7 is due to the first helium ionization. There is an OPAL enhancement around LogT=6.3. However, this apparent large increase in opacity is due to a limitation of the Stellingwerf fits. A direct comparison to the actual Cox-Tabor (1976) tables only leads to opacity enhancements of 30% in the LogT≈6.3 region as shown in Fig. 5. These modest opacity increases can affect helioseismology and lithium burning rates and is due both to improved atomic physics and EOS.

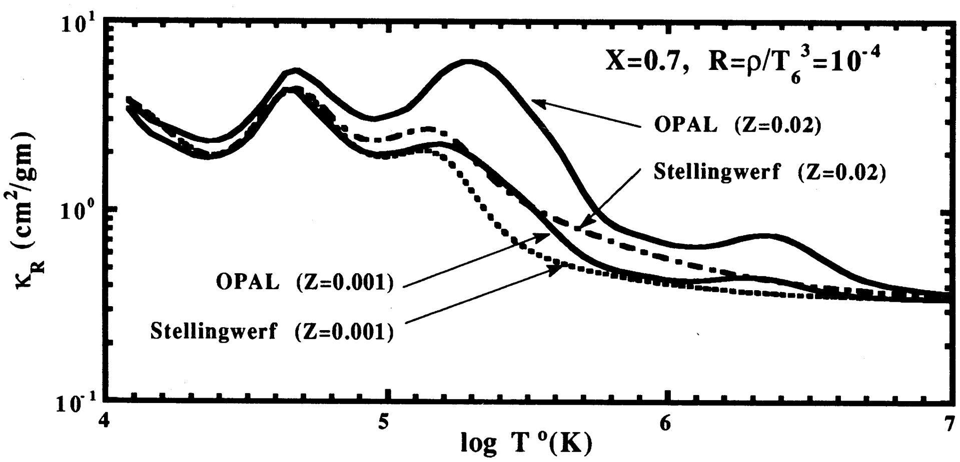

Figure 4 --- OPAL opacities and Stellingwerf fits for hydrogen mass fraction X=0.7 with metallicity Z=0.001 and Z=0.02. Here, $R=\rho/T_6^3$ where ρ is in gm/cm^3 and T_6 is temperature in millions of degrees.

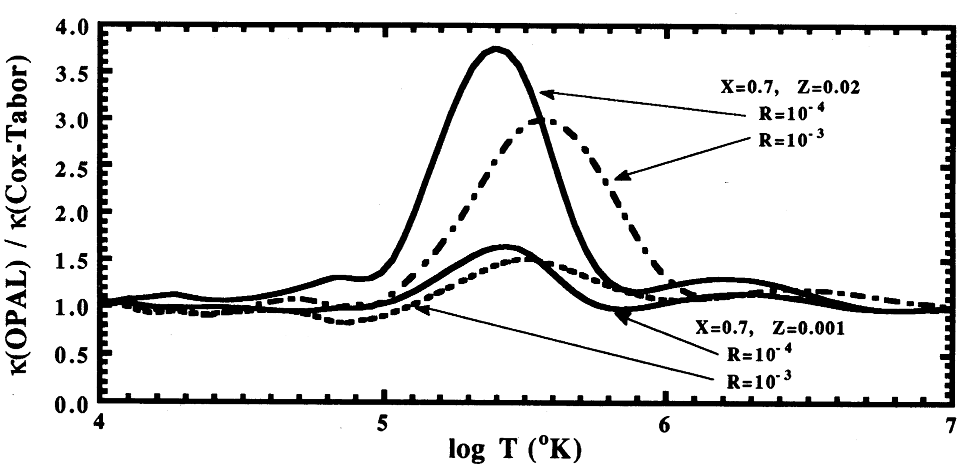

Figure 5 --- Ratio of OPAL to Cox-Tabor opacities for Z=0.001 and Z=0.02 for values of $R=10^{-3}$ and $R=10^{-4}$. These values are typical of classical Cepheid and RR Lyrae stellar pulsation models.

In Figs. 4 and 5 the region near LogT≈5.4 shows a large OPAL opacity enhancement due to improved atomic physics. In particular, the hydrogenic oscillator strengths used by Los Alamos in their bound-bound spectrum is a poor approximation for complex ions since they do not predict any $\Delta n=0$ transitions (transitions between the same principal quantum number) which, in fact, produce strong absorption features. In addition, the configuration term splitting, which is almost completely absent in the Los Alamos codes, replaces single, narrow spectral lines (these contribute little to the Rosseland mean opacity) with many weaker lines spread out over a significant energy range.

In Figs. 6 and 7 the frequency dependent coefficient for iron is presented with and without the configuration term splitting. Although the difference in the individual iron opacities between Figs. 6 and 7 is more than a factor of 30, due to the small iron abundance the opacity for the mixture is only increased by approximately a factor of 3. This is shown in Fig. 5 where the ratio of OPAL to the Cox-Tabor (1976) opacities is plotted. Note that the difference in Planck means between the iron results in Figs. 6 and 7 is in the order of 10%. That is, the total photon absorption strength is, as expected, approximately conserved. The small difference can be attributed to line shifts and occupation number differences due to the configuration term splitting and its effect on the Boltzmann factors.

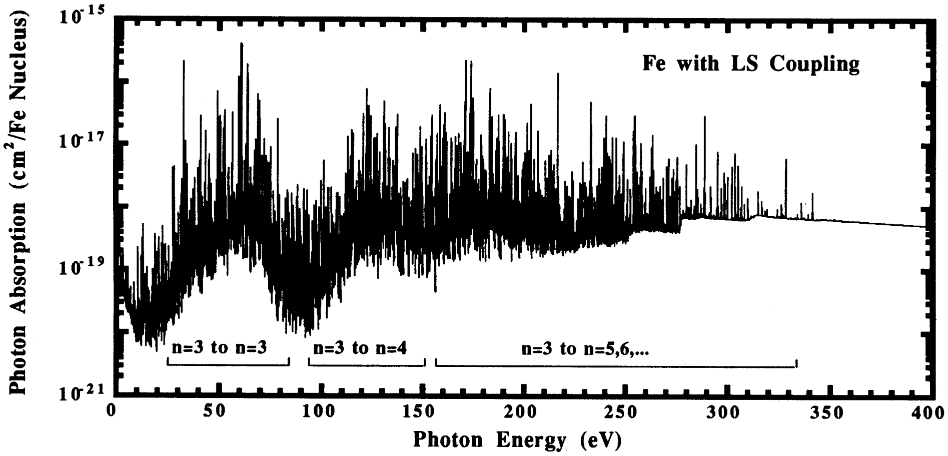

Figure 6 --- Photon absorption coefficient as a function of photon energy for iron in a mixture with X=0.7 and Z=0.02 at LogT=5.4 and LogR=-3.5. Spectral lines computed in the LS-coupling scheme.

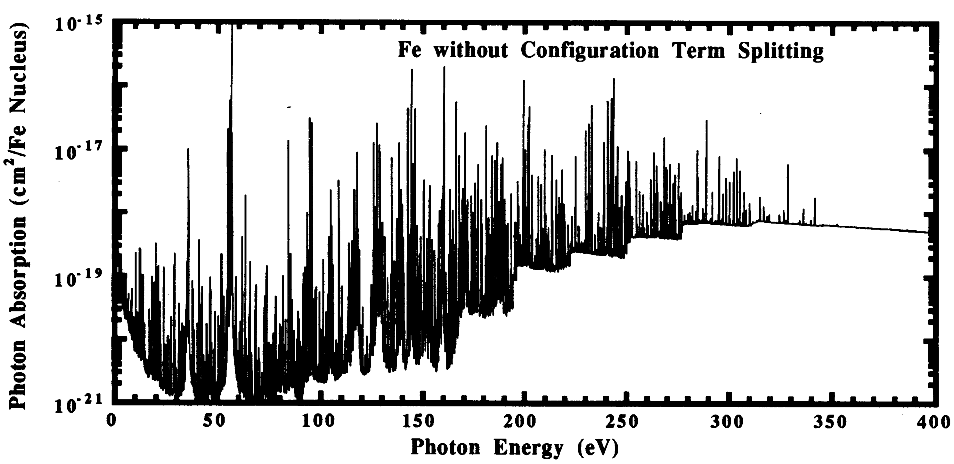

Figure 7 --- Same as Fig. 5, but without configuration term structure.

Clearly, the opacity enhancements from OPAL could have a significant effect on pulsation models. Recently, Moskalik, Buchler, and Marom (1992) (also see Simon and Kanbur, this Volume) have greatly reduced the so-called beat and bump mass discrepancies in multimode Cepheids. In addition, their non-linear modelling with OPAL opacities led to good qualitative agreement with observed Cepheid light and velocity curves. Application of the OPAL opacities in RR Lyrae models has also lead to a resolution of the mass discrepancy for these extremely low metallicity stars (Kovacs, Buchler, and Marom, 1992). In this case, however, an opacity enhancement as well as an opacity decrease near LogT=4.5 of approximately 10-20% was responsible (Cox 1991). The opacity decrease in OPAL relative to Los Alamos has been traced to an improved treatment of the Lyman-alpha line wing of hydrogen (Rogers and Iglesias 1992).

III.c *Lithium Abundance*

Swenson, Stringfellow, and Faulkner (1990) have proposed that the long standing disagreement between the depletion pattern observed amongst the Hyades G-dwarfs, can be resolved if the Los Alamos interior opacities underestimate the true values. The new OPAL opacities were utilized in their lithium burning model and they found that the results go a long way towards resolving the lithium depletion problem in the Hyades (Swenson, Faulker, Iglesias, and Rogers 1991). The preliminary results using OPAL opacities are shown in Fig. 8 and are compared to results using the Cox and Tabor (1976) opacity tables. Note that the large lithium depletion near $T_{eff} = 6650K$ is a distinct problem which can be explained by diffusion phenomena and involves a competition between radiation pressure and gravitational settling in these slightly hotter but more stable stars.

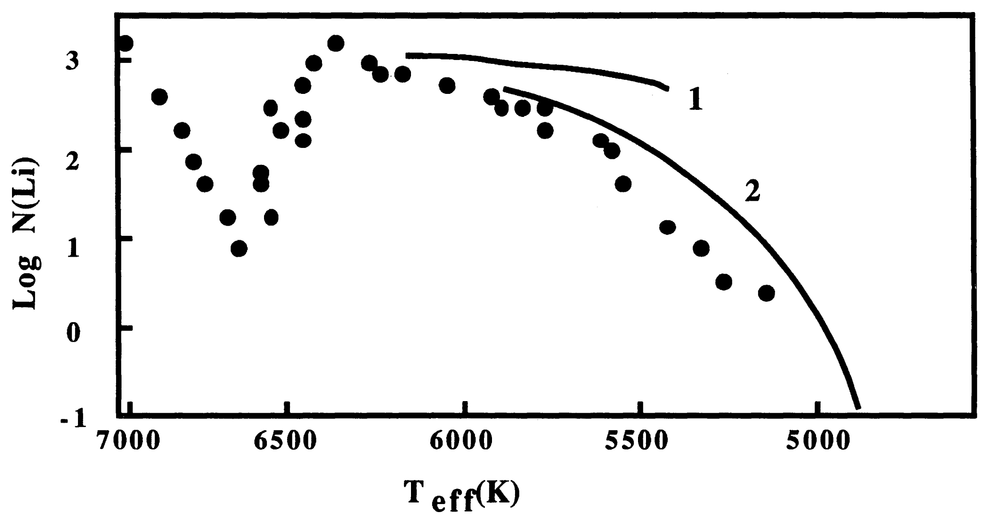

Figure 8 --- Lithium abundances are plotted versus star surface temperatures where the initial value is Log N(Li)=3.2 and the scale Log N(hydrogen)=12 is used. Curve 1: Cox and Tabor (1976) ; Curve 2: OPAL ; •: observations.

IV. CONCLUSION

The OPAL code removes several approximations made in previous opacity calculations. The EOS approach avoids the *ad hoc* cutoffs and intuitive arguments present in free energy minimization schemes. The parametric potential model offers reasonably accurate atomic data (e.g., a few percent error in configuration-averaged energies compared to experiment). Furthermore, OPAL includes configuration term splitting (in the LS-coupling scheme) which considerably increases the number of spectral lines; thus, filling in spurious "windows" in the absorption coefficient and restricting the flow of photons.

The improvements in atomic physics lead to a large opacity enhancement over past calculations at $T \approx 3x10^5$K. There can be no doubt that this OPAL opacity enhancement due to the metals is real. However, due to the very complex nature of the atomic physics and line broadening theories involved in the photon absorption calculation of ions with partially filled M-shells, the precise magnitude of the enhancement must be regarded as somewhat uncertain. Although sensitivity tests were not given in the present discussion, uncertainties in the metal opacity are provided in Rogers and Iglesias (1992).

At higher temperatures, $T \approx 3x10^6$K, modest opacity enhancements of 10-30% are noted which can affect helioseismology as well as lithium depletion. For low densities, these larger opacities at the hotter temperatures are probably due to improved atomic physics (Rogers and Iglesias 1992). At higher densities the enhancement is due to EOS issues (Iglesias and Rogers 1991a).

Certainly, other problems in astrophysics will need to be addressed with the new OPAL opacities. The problem of convection overshoot could be significantly affected by the new opacities (Stothers 1991). The mass-luminosity relations should be computed. As more is learned about the effect of the new opacities, new problems will arise. For example, the OPAL opacities show a sensitivity to the metal mass fraction not present in previous calculations Hence, the pulsation instabilities associated with it should display sensitivity to the metallicity absent in previous stellar models and possibly subject to stellar observations.

In Rogers and Iglesias (1992) opacity tables are given for the Anders-Grevesse (1989) metal composition which extend to low enough temperatures to allow a smooth transition into other tables which include molecular absorption coefficients (recall OPAL does not have molecular photoabsorption). The density and temperature covered by the tables should be sufficient for a broad range of astrophysical applications. However, a number of important issues cannot be addressed. For example, the opacity tables allow for changes in metallicity, Z, but not for changes in the relative metal abundances (except for the few tables with Cox-Tabor and Ross-Aller mixtures). Requests for compositions with different metal abundances can easily be satisfied. The reason is that we can take advantage of the fact that the EOS is dominated by H and He so that occupation numbers are insensitive to changes in the abundance of an individual metal. Therefore, we can re-mix the individual element frequency-dependent photon absorption coefficients computed assuming the Anders-Grevesse composition to obtain the Rosseland mean opacity of a new mixture with different relative metal abundances but fixed X and Z.

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