Update of MEKA: MEKAL

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1. Introduction

The analysis of the X-ray spectrum of the Centaurus cluster as measured with the ASCA satellite by Fabian *et al.* (1995) has demonstrated that the observed intensity distribution in the dominant Fe L-shell feature around $\sim$ 1–1.5 keV is not consistent with the predictions of the commonly used optically thin plasma codes such as Raymond-Smith and MEKA. In particular the observational data indicate a higher value than the plasma models predict of the ratio Fe $(3 \rightarrow 2)/(4 \rightarrow 2)$ of the two line complexes $n = 3 \rightarrow n = 2$ and $n = 4 \rightarrow n = 2$ at about 1.1 and 1.5 keV, respectively. Such a discrepancy could not be removed by varying the relative metal abundances nor by invoking a multi-temperature distribution (cf. Fabian 1994, Fabian *et al.* 1995).

1) Though the ASCA observations with a modest spectral resolving power of about 20 in this region permit the separation of the two blended components, they do not allow the resolution of the fine structure of each of these Fe L components which are composed of thousands of lines from ions in the range Fe XVII–XXIV that are formed in the temperature region $6.5 \lesssim \log \mathrm{T(K)} \lesssim 7.3$. Though the current models, which have concentrated only on the stronger lines (nearly 250 in total), still give a good order-of-magnitude estimate of the fluxes, more detailed calculations are now required to reproduce the observed structure in the Fe L-shell complex for the broad-band ASCA observations and even more detailed calculations are needed for the high-resolution XMM and AXAF spectra.

These problems have motivated us to make use of recent calculations of the Fe L complex with the HULLAC code at Livermore and to implement the results in an upgrade of our previous plasma code, that was installed end 1992 in the latest release of XSPEC (version 8.23) under the name MEKA (cf. Kaastra & Mewe 1993, Mewe & Kaastra 1994). Some preliminary calculations by Liedahl *et al.* (1994) using about 1000 of the strongest lines from Fe XXII–XXIV as calculated with HULLAC showed that a revision was warranted. Some more detailed computations by Liedahl *et al.* (1995) have confirmed this.

2) Our experience with the data analysis of EUVE spectra of cool stars (Mewe *et al.* 1995) has led us to make some revisions to the list of lines of Landini & Monsignori Fossi (1990) that we used since 1992 for the extension to the 300–2000 Å wavelength region. We modified several excitation rates, corrected the wavelengths of about 110 lines between 80–500 Å, while in

a dozen of cases we have split up the average multiplet into its separate components.

3) Discrepancies in the comparison between observations of the diffuse emission from the hot ISM with the Diffuse X-ray Spectrometer (DXS) in the 44–84 Å range and currently used spectral models (Sanders 1995) has led us to recalculate the lines from Fe VIII to Fe XVI in the wavelength region ∼35–2000 Å using data from the literature for collision strengths and radiative branching ratios.

4) Finally, we added a number of dielectronic recombination (DR) satellites to the He-like Mg lines at 1.3 keV and use the Arnaud-Raymond (1992) ionization balance for Fe instead of the Arnaud-Rothenflug (1985) ionization balance which is still used for the other elements.

To summarize, the forthcoming release of MEKA under the name 'MEKAL' contains the following improvements:

(i) improved calculations of the Fe-L complex between 0.65–1.83 keV based on the HULLAC results; (ii) addition of about 300 far-UV lines between 300–2000 Å from Landini & Monsignori Fossi (1990) with some lines corrected for excitation rates and wavelengths and/or splitted in multiplets based on the analysis of EUVE spectra; (iii) update of Fe VIII–XVI lines in the 35–1950 Å region; (iv) addition of about 60 DR lines to the He-like Mg lines at 1.3 keV; (v) Arnaud-Raymond (1992) ionization balance for iron.

2. Calculations of the Fe L-shell spectrum

In calculating the Fe L-shell spectrum one of us (DAL) has used the atomic physics package HULLAC (Hebrew University/Lawrence Livermore Atomic Code) developed by Klapisch and co-workers (Klapisch 1971, Klapisch *et al.* 1977). Excitation collision strengths are calculated in the quasi-relativistic distorted wave approximation (Bar-Shalom *et al.* 1988). Results for Fe XXIV are within a few percent in agreement with the results by Zhang *et al.* (1990) computed in the relativistic distorted wave approximation.

At the moment more than 40 0000 lines have been calculated from the ions Fe XXI–XXIV and calculations for the remaining ions Fe XVII–XX are in progress. The energy-dependent excitation Gaunt factor parameter method as originally proposed by Mewe (1972) and Mewe & Schrijver (1978) was used for the calculation of line emission in the MEKA code. Our newer work extends this idea by introducing, apart from Mewe's formula for the majority of the lines, different fitting formulae for other lines, in particular forbidden transitions. These results will, apart from a higher accuracy, also

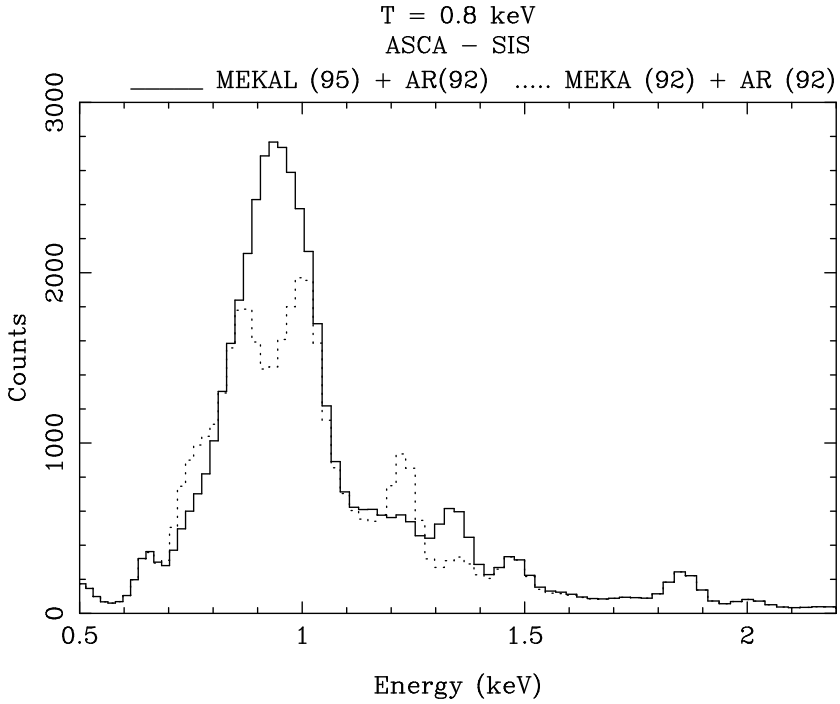

Figure 1: Spectrum simulated for the ASCA-SIS for a temperature T = 0.8 keV using MEKAL with Arnaud-Raymond (1992) ionization balance for iron and Arnaud-Rothenflug (1985) ionization balance for the other elements (solid line) or using MEKA with the same ionization balances (dotted line).

allow the calculation of the density dependence of the Fe L and Fe M shell lines.

However, for the implementation in MEKAL on a short term we have still used the old formalism but we have extended and improved our line list by implementing the 2300 of the strongest lines calculated by the HULLAC code for the wavelength region 6.8–19.0 Å from the ions Fe XVII–XXIV including the 3-2 and 4-2 lines, and sometimes also 5-2 lines. For Fe XXIII also the effects of dielectronic recombination (DR) were included. In more extended calculations for Fe XXIII and Fe XXIV by Liedahl *et al.* (1995) also radiative recombination (RR) was taken into account. In the present calculations we have calculated the contribution of RR to the strength of lines from the ions Fe XXIII and Fe XXIV in an approximate way by using Eqs. (33)–(35) from Mewe & Gronenschild (1981). The contribution from DR for the ions Fe XVII–XXII and Fe XXIV we have taken approximately into account by using Eqs. (43)–(45) from Mewe & Gronenschild (1981) for the estimate of the total intensity of satellites close to a resonance line. Note that Eq. (43) contains a printing error: the constant should be 8.133×10^{-13} instead of

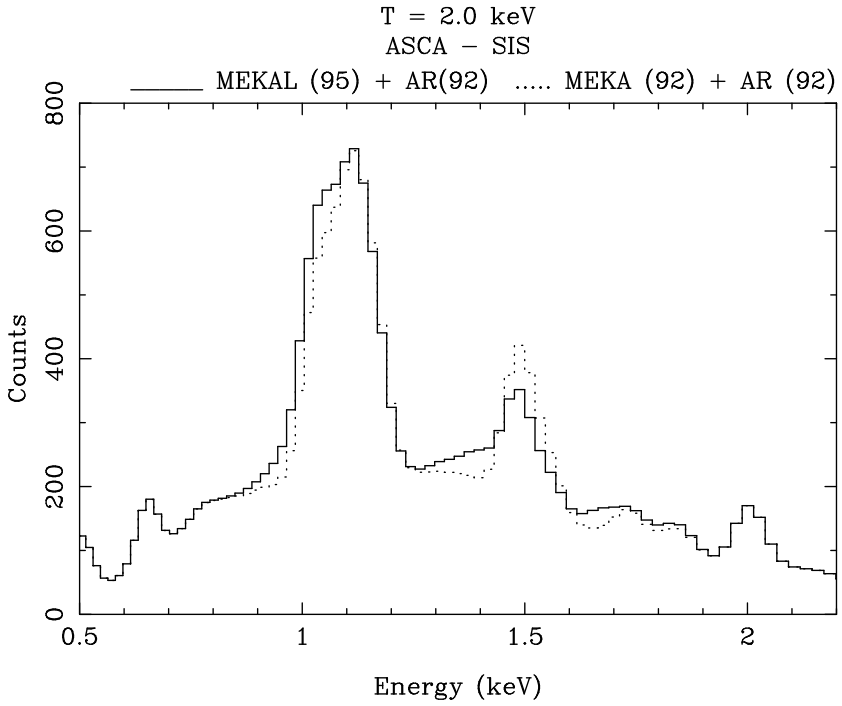

Figure 2: The same as Fig. 1 but for T = 2 keV.

8.14×10^{-14}; note also that the electron temperature $T_{\rm e}$ is expressed in units of 10^6 K and the excitation energy χ_z^E in eV.

The total number of lines in the Fe L spectrum between 6 and 20 Å included in MEKAL is 2652 as compared to 244 in MEKA.

2.1. Comparisons and conclusions

Figs. 1 & 2 compare simulated X-ray spectra for the ASCA-SIS with the new MEKAL and the old MEKA for the temperatures 0.8 and 2 keV using AR92 for Fe and AR85 for the other elements. A few differences are noticed. At T = 0.8 keV the peak in the spectrum shifts from $\sim$ 1 keV (from Fe XXI) in MEKA to a larger peak at $\sim$ 0.9 keV (from Fe XIX) while the Fe XX feature at 1.23 keV shifts to 1.31 keV. The features at 1.47 keV and 1.85 keV are dominated by Mg XII and Si XIII emission, respectively. At T = 2 keV the peak at 1.1 keV is determined in both codes by Fe XXIV lines but shows for MEKAL a low-energy 'shoulder' due to Fe XXIII emission. In MEKAL the 'gap' between 1.3–1.4 keV is filled by Fe XXII lines. Mg XII emission still gives a significant contribution to the $\sim$ 1.5 keV blend while the 2 keV emission is entirely due to Si XIV. Figs. 3 & 4 show, apart from different line excitation calculations, the use of different ionization balances for iron

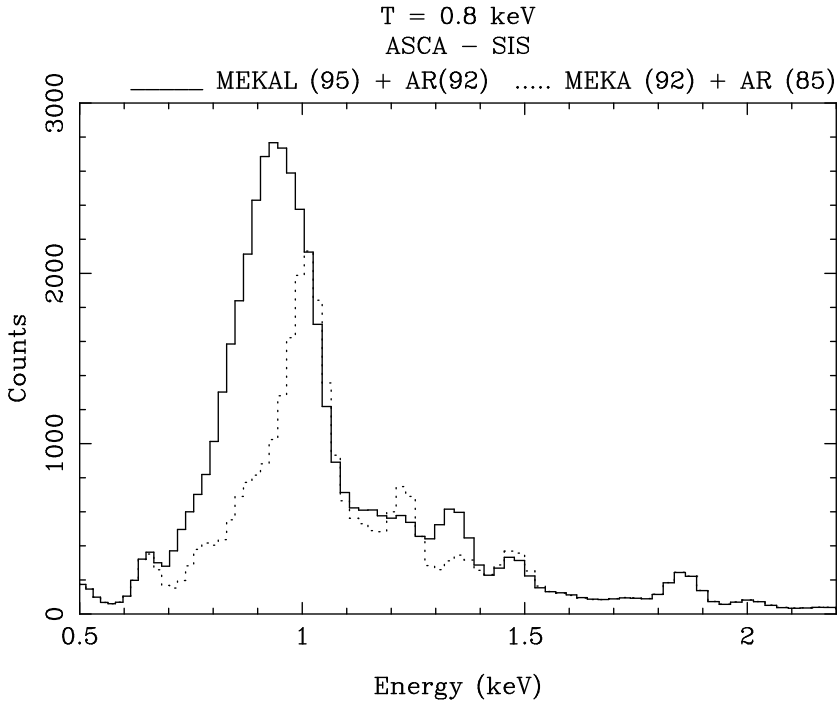

Figure 3: The same as Fig. 1 but for MEKA now Arnaud-Rothenflug (1985) ionization balance was used also for iron.

(AR92 in MEKAL vs. AR85 in the original MEKA code). The last two plots show the full difference between the MEKA and MEKAL calculations and show evidence that the new calculations significantly enhance the 3-2/4-2 ratio due to the combined effects of line excitation and ionization balance (cf. also Liedahl *et al.* 1995). However the contributions from e.g. Mg XI and Mg XII emission to the '4-2' blend can not be neglected in the considered temperature range.

3. Calculations of Fe VIII–XVI

On the basis of data taken from the literature for excitation collision strengths and radiative branching ratios we have revised the intensities from the lines of the ions Fe VIII–XVI in the wavelength region 35–1960 Å for the low-density case. The results for Fe XII and Fe XVI we have checked in personal correspondence with the calculations by Nancy Brickhouse. For the dependency on electron density of the long-wavelength ($\gtrsim$ 80 Å) lines of these ions we refer to her calculations (Brickhouse *et al.* 1995). The total number of lines from these ions increased from 245 in MEKA to 477 in MEKAL.

4. SPEX

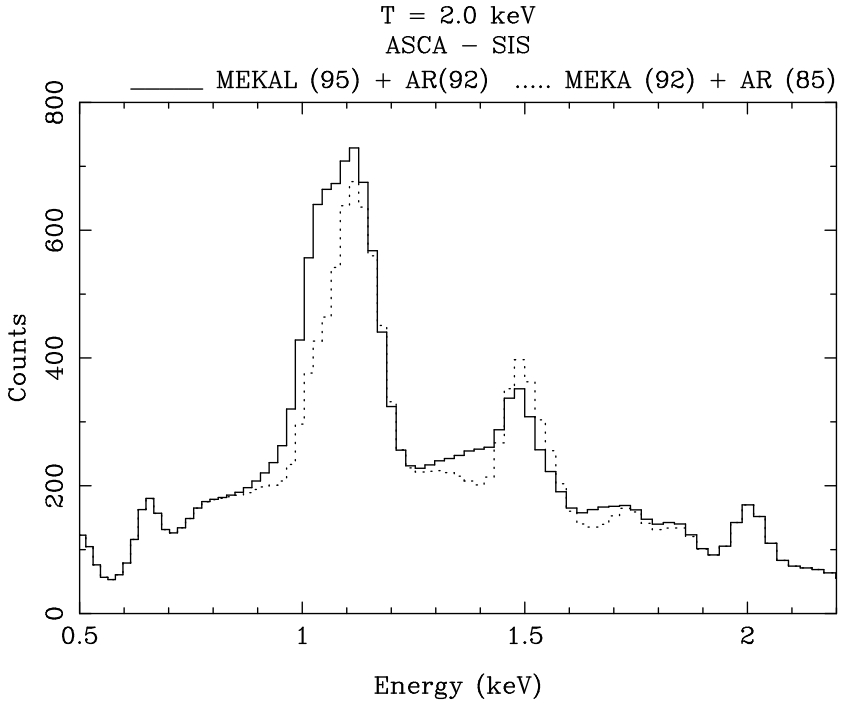

Figure 4: The same as Fig. 3 but for T = 2 keV.

More extended calculations with the HULLAC code of the Fe L complex and also long-wavelength lines of these ions are in progress. New model calculations for the wavelength range $\sim$ 1–2000 Å, will include non-equilibrium ionization, photo-ionization, X-ray absorption, and density effects. These and hydrodynamical models for extended sources like supernova remnants and clusters of galaxies, multi-temperature (DEM) models, including extended diagnostic and display facilities, will become available in our new spectral code SPEX (cf. Mewe & Kaastra 1994).

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