Abstract. It is desirable to calculate the X-ray emission spectrum from a (region of a) plasma that is not in ionization equilibrium, e.g., with application to supernova remnants, SNRs. Such a plasma will generally have ionization fractions that are not directly related to the local electron temperature and, in the case of SNR ejecta, may contain little or no H and He. This work describes the use of a currently available database, ATOMDB, and software, ISIS, to generate spectra for a non-equilibrium ionization, NEI, plasma which is specified by explicit densities and ionization fractions and an independent electron temperature. An example spectrum is shown and discussed. The approach here does have some deficiencies currently: not all relevant inner-shell lines are included, there are no Cr lines, and continua spectra are not given on an ion-by-ion basis. Finally, in the low density, NEI case, it may be useful to consider the emission components that arise from each "quiescent" ion.

Keywords: atomic processes, hydrodynamics, plasmas, radiation mechanisms: thermal, supernova remnants, X-rays: ISM

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There are many cases where it is desirable to calculate the X-ray emission from a plasma that is not in collisional-equilibrium ionization, CEI. We have for example: the outputs of hydrodynamical models of Type Ia supernova remnants, SNRs[1], the emission from specific knots in a Type II SNR[2], the idealized models such as a plane parallel shock or a Sedov blast wave, and even the case of \textit{ab initio} models where the plasma is simply built to agree with observational data. In all these cases the specifics of the plasma are known and the resulting X-ray spectrum is desired.

FIGURE 1. 2D projections of Type Ia ejecta models. Badenes et al.[1] models DDTa (left) and DDTe (right) are shown at $t = 1000$ yr. The image color values, R:G:B, are determined by the element column densities of Fe:Si:Ni; e.g., the colors indicate: blue-Ni, purple-Fe+Ni, red-Fe, orange-Fe(+Si), yellow-Si+Fe, green-Si. The image brightness is weighted by $n_e$, emphasizing ionized regions.
Here we apply current CEI atomic data and software to approximate emission from a non-equilibrium ionization, NEI, plasma. As a specific example we use the models of Badenes et al.\cite{1} which describe Type Ia SNR ejecta. These are 1D hydrodynamical models of 3D spherically symmetric explosions and give the plasma composition and properties in discrete shells or layers as a function of time. The images in Figure 1 show visualizations of the composition variation for two different models. The goal inspiring this work is to calculate and visualize the X-ray emission from such a model.

Given model parameters, in this case for each layer or spherical shell of the Type Ia model, Figure 2, we can convert them into parameters used by standard codes; here we use the Interactive Spectral Interpretation System, ISIS\cite{3} and the ATOMDB spectroscopy database\cite{4}. Using as an example layer 90 of a DDTe model at 1000 yr. for which $T_e \approx 14$ MK, the norm and the abundances are determined. This layer’s elemental abundances expressed with respect to “solar” are found to be in the range of 500–3500 for Si, S, Ar, Ca, Cr, and Fe. Note that these equivalent abundances are based on the electron density: $A_z = (n_z/n_e)_{\text{model}}/(n_z/n_e)_{\text{solar}}$ so that the presence of H and He is not assumed. Likewise the value of $n_e$ is self-consistent with the densities and ionization states of the plasma’s ions, i.e., $n_e = \sum_z n_z \bar{q}_z$.

It is straightforward to calculate the modified-abundance CEI spectrum for this layer, shown by the light curve in Figure 3. The final step in generating the spectrum is to include the effect of the actual ion-fractions by scaling the line emission from each ion by the ratio of the assumed CEI ion fraction to the desired model ion fraction. The difference between CEI and NEI ion populations at the same temperature can be large—for this layer over 80% of the NEI model Si atoms are in the ion states Si IX, Si X, and Si XI; whereas the CEI case has $>99\%$ of the Si atoms in Si XIII and higher ionization states. As might be expected, the final NEI spectrum, the dark curve in Figure 3, has very little K-shell emission from the elements present, i.e., shortward of 7 Å.

Clearly this approach currently has some deficiencies, most importantly the lack of inner-shell lines from low-ionization states, e.g., Si-K-shell lines from Si X in the presence of high-T electrons. Relatedly, the continua would ideally be given on an ion-by-ion basis as well. Of relevance to the Type Ia models, Cr lines are not currently in ATOMDB. Finally, in the low density, non-equilibrium case considered here, it may be useful to consider, tabulate, and label the emission components that arise from each
FIGURE 3. Example of an NEI spectrum. The spectrum for layer 90 of the DDTe 1000 yr. model is shown (light,pink) assuming CEI conditions for $T_e \approx 14$ MK. Scaling by the actual model ion fractions gives the spectrum (dark,green) dominated by lines in the 10–17 Å range.

“quiescent” ion population as opposed to the actual emitting ion which may only form as a result of an interaction, e.g., one of the “three fundamental binary electron-ion collision processes” [5]. In this way Si X would be seen as the parent of “Si IX lines” via dielectronic recombination, and O IX would be viewed as the source of some “O VIII” emission; in each case, the emission scales with the quiescent parent ion population.

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