Isotopic Fractionation in $^3$He-rich SEP Events

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Abstract. A well established characteristic of $^3$He-rich solar energetic particle events is a pattern of abundance enhancements relative to normal solar system values that increase approximately monotonically with atomic number (or mass), leading to enhancements that can exceed $100 \times$ for the heaviest elements relative to oxygen. In a 2018 paper, Mason and Klecker (M&K) suggested that the heavy element enhancements could be due to characteristics of the stopping powers of low-energy nuclei penetrating thin layers of H gas or plasma. We present results of a new calculation of enhancements in a H gas and show them to be in reasonable agreement with the M&K results. Studies of heavy-element isotopic composition in $^3$He-rich events using data from ACE/SIS have also shown that heavier isotopes of an element typically exhibit significant abundance enhancements relative to lighter isotopes of the same element. We applied the new calculation to investigate whether the observed isotopic fractionation can be explained using the M&K H-gas model with the same parameters that account for the heavy-element abundances and found that the measured isotopic enhancements are significantly greater than the predicted values. A search of a larger parameter space was also not able to reconcile the elemental and isotopic enhancement values. However, this search did reveal trends in the dependence on the model parameters that merit further investigation.

1. Introduction

Impulsive solar energetic particle (SEP) events are characterized by enhancements of $^3$He/$^4$He by several orders of magnitude over the solar wind value of $\sim 4 \times 10^{-4}$ [1] and a pattern of heavy element enhancements that increases approximately monotonically with the atomic number (or the mass) of the element, with Fe/O typically enhanced by $\sim 10 \times$ and with enhancements of the heaviest elements relative to O that can reach $\sim 100 \times$ or more [2, 3]. Studies have shown [4] that the heavy element enhancements have little, if any, correlation with the enhancements of $^3$He/$^4$He in the same events, leading to the strong suspicion that two different mechanisms are responsible. A number of authors argued that the $^3$He enhancement results from the resonant interaction of this nuclide with some type of plasma waves that heat only this ion, which has a mass-to-charge ratio, $M/Q$, far from that of all other nuclides commonly observed in these events (e.g., [5]). The mechanism responsible for the heavy-element fractionation has lacked a compelling, quantitative explanation for more than four decades.

Mason & Klecker [6] (henceforth M&K) showed that the pattern of heavy element enhancements can be produced by a simple mechanism associated with the effective atomic charge that low-energy, heavy elements attain when slowing down in matter, taking into account both ionizing and non-ionizing energy losses. As a result of the relatively larger number of orbital
electrons attached to an Fe nucleus than to an O nucleus at equal values of their energy per nucleon \((E/M)\) below \(\sim 1 \text{ MeV/nuc}\), Fe is more penetrating than O.

M&K showed that if power-law energy spectra of the elements are incident on a thin layer of hydrogen gas and only those particles that penetrate the layer are further accelerated, the layer can act as a filter that modifies the relative abundances of the elements. Values were found for the power-law spectral index, \(\gamma\), and the material thickness ("grammage", defined as thickness \(\times\) mass density) of the layer, \(L\), such that this filter did a reasonable job of reproducing the observed pattern of heavy-element enhancements \([2, 3]\), at least over the mass range \(4 \leq M \leq 100\) (corresponding to elements with \(2 \leq Z \leq 50\)).

M&K also reported that the same mechanism operating in the more realistic environment of hot hydrogen plasma, such as would be encountered in the solar corona, can produce a similar enhancement pattern, albeit with different parameters and larger uncertainties in the calculation.

Measurements of heavy-element isotopic composition in \(^{3}\text{He}\)-rich SEP events and their correlations with one another and with the Fe/O enhancement \([7, 8, 9, 10]\) provide additional probes of the fractionation mechanism. Characteristically, the heavier isotopes of an element are enhanced relative to the lighter isotopes of that element. For the heavy isotope ratio, \(^{22}\text{Ne}/^{20}\text{Ne}\), enhancement factors exceeding \(\sim 3\times\) are not unusual.

In this paper, we further test the M&K model for the case of a medium consisting of neutral H gas. In Section 2, we summarize the key features of the model and describe a new calculation. In Section 3, we apply the model to the calculation of the elemental abundance enhancement pattern using parameters favored by M&K and show that this new calculation does a reasonable job of reproducing results found by M&K. We then apply the model with these same parameters to the calculation of isotope ratio enhancements and compare the calculated values with measurements from ACE/SIS \([9, 10]\). We find that these parameters do not account for isotope ratio enhancements as large as have been observed. We then discuss the search of a larger range of parameter space to find parameters that can account for the isotopic and elemental enhancements. We show that more extreme power-law spectra are required to account for the observations of \(^{22}\text{Ne}/^{20}\text{Ne}\), particularly if the model is to simultaneously account for measured Fe/O values. In Section 4 we discuss the model predictions for the correlations between enhancements of \(^{22}\text{Ne}/^{20}\text{Ne}\) and \(^{26}\text{Mg}/^{24}\text{Mg}\) and between \(^{22}\text{Ne}/^{20}\text{Ne}\) and Fe/O. We find that the enhancement factors for these ratio pairs are nearly proportional and are only weakly dependent on the actual values of the model parameters used to account for the observations. In Section 5 we discuss the need to extend the isotope calculations to the case of energy loss in a hot plasma, as done by M&K for element enhancements, and the complications that need to be addressed to do so. In Section 6 we summarize the key results of this study.

2. Calculation of Abundance Ratio Enhancements

We used version 10.3 of the Geant4 simulation package\(^1\) \([11, \text{ and references therein}]\) to replicate calculations reported by M&K, which were based on the widely used “The Stopping and Range of Ions in Matter” (SRIM) package\([12]\). Primary nuclei with specified atomic number \((Z)\), mass number \((M)\), and initial kinetic energy per nucleon \((E/M)\) were injected at the center of a large volume of hydrogen gas at standard temperature and pressure. The software followed the energy loss and interactions (e.g., knock-on electron production) in a series of steps until each nucleus came to rest. The total distance travelled while slowing down and also the projection of that distance on the direction of the particle’s incident velocity were recorded. For each primary beam, a large number of nuclei were followed in order to derive the range and projected-range distributions. Figure 1 shows the range–energy relations for \(^{16}\text{O}\) and \(^{56}\text{Fe}\) (righthand panel) and the corresponding dependence of the specific ionization per nucleon on \(E/M\) obtained by

\(^1\) The Geant4 physics option emstandard_opt3 was used.
differentiation (lefthand panel). The crossover at low energies, which is evident in both plots, is the basis for the fractionation effect proposed by M&K.

![Figure 1. Dependence of $d(E/M)/dx$ (left) and $R$ (right) on $E/M$ obtained from the Geant4 model.](image)

For selected nuclides, the upper panel of Figure 2 shows with solid bars the $E/M$ intervals over which essentially all particles incident on a H gas layer of thickness 200 $\mu$g/cm$^2$ would penetrate the layer and with hatched bars the $E/M$ intervals over which range straggling would cause only a fraction of the particles to penetrate. At still lower energies, all of the particles would stop in the layer. For comparison, the lower panel of Figure 2 illustrates power-law energy spectra that could be incident on the H gas layer for several values of the spectral index, $\gamma$. As a result of energy losses in the H layer, the energy spectra of the exiting particles (not shown) are significantly distorted from the incident spectra and extend all the way down to zero energy. However, if all of the transmitted particles subsequently undergo acceleration independent of the energies they had when exiting from the absorber, this distortion of the spectral shape will not affect the fractionation. This is the case considered by M&K and by us. On the other hand, if there is an energy threshold below which particles exiting the layer are not accelerated, then the shape would matter.

Comparing $^{56}$Fe with $^{16}$O, the partial-transmission regions are well separated from one another. For the power laws that are shown, the selection of only penetrating particles for acceleration results in a significant excess of Fe relative to O. Comparing the isotopes $^{20}$Ne and $^{22}$Ne, the partial-transmission regions are much closer together, so to obtain a large enhancement of $^{22}$Ne/$^{20}$Ne requires a steep (soft) power law.

It is notable that for two isotopes of the same element, the heavier isotope should always have the longer range at any specified $E/M$. Thus, one expects that the fractionation will always favor the heavier isotopes. This is the pattern observed in the data [8, 9, 10].

When the incident power law is very steep, there can be a significant variation of the incident flux even over the rather narrow region of partial transmission. For this reason, we mapped out the partial-transmission region in considerable detail, finding the $E/M$ values at which 1%, 2%, ..., 99% of the incident particles make it through the layer. Let $R_{Z,M}^{Z,M}(E/M)$ denote the grammage for which a fraction $f$ of the particles of a particular nuclide $Z,M$ and incident energy $E/M$ are transmitted. We simulated 1000 particles for each of a series of incident beams with
Figure 2. Upper panel: $E/M$ intervals over which beams of selected nuclides penetrate a layer of H of grammage 200 $\mu$g/cm$^2$ either completely (solid section) or partially (hatched section). Lower panel: Example power-law incident spectra with selected values of the spectral index, $\gamma$.

300 logarithmically spaced $E/M$ values per decade (step size of 0.77%) from 0.01 to 10 MeV/nuc and used the resulting projected ranges to determine $R^{Z,M}_f(E/M)$ for $f = 0$ to 1 in steps of 0.01 for each of the simulated $E/M$ values. To find $R^{Z,M}_f(E/M)$ for values of $E/M$ that were not simulated, we interpolated between adjacent $E/M$ values at equal $f$.

The relative numbers of transmitted particles for two different nuclides with a given incident power-law spectrum, $(E/M)^{-\gamma}$, was calculated by adding the analytically calculated integral over the region for 100% transmission to the numerically calculated integral over the region of partial transmission and taking the ratio of the integrals for the two nuclides. This ratio gives the relative enhancement of the two nuclides. It is noteworthy that for steep incident spectra the population of transmitted particles is dominated by those with energies close to the threshold for penetration. Conclusions about the enhancements of abundance ratios should be applicable as long as the spectrum can be reasonably approximated by a power law between the penetration thresholds for the two species.

3. Elemental and Isotopic Enhancement Patterns
The lefthand panel of Figure 3 shows the pattern of elemental abundance enhancements that we obtained and compares them to measured values [2]. They are generally consistent with the calculations of M&K for the same parameters. The righthand panel of the figure shows our calculation of various isotope-ratio enhancements for the same set of parameters. The comparison with measurements from the 2002 Aug 20 $^3$He-rich event [10] shows that the observed isotope enhancements significantly exceed those that would be expected from the model that reproduces the elemental values.

We examined a wider range of spectral indices for the same grammage (200 $\mu$g/cm$^2$) to see if
Figure 3. Left panel: Pattern of elemental abundance enhancements calculated for the grammage of 200 \(\mu g/cm^2\) of H gas used by M&K and four values of \(\gamma\), the index of the incident power-law spectrum (blue curves). Red points show measured values from \[2\]. Dashed vertical line indicates the Fe point. Right panel: Isotope ratio enhancements versus mass ratio. Blue curves calculated using the same model parameters as used for the left panel. Red points show measured values from \[10\] labeled with the nuclide in the numerator of the ratio. The denominator in each case is the most abundant isotope of the same element. Dashed line shows power-law fit to the isotope data from the 2002 Aug 20 event \[10\].

The isotope enhancements could be accounted for, independent of the elemental enhancements. The lefthand panel of Figure 4 shows the resulting comparison for a spectral index \(\gamma = 9.0\). The model results account for the observations at least as well at the simple power-law dependence on the mass ratio that was presented by \[10\], which is shown by the dashed line in Figures 3 and 4. The deviations from a simple power law are an interesting feature of the model. However, it should be noted that in two cases where values are available for identical mass ratios (\(^{22}\)Ne/\(^{20}\)Ne and \(^{44}\)Ca/\(^{40}\)Ca with a ratio of 1.100 and \(^{13}\)C/\(^{12}\)C and \(^{26}\)Mg/\(^{24}\)Mg with a ratio of 1.083), the isotope ratio that shows a larger enhancement in the data is predicted to have a smaller enhancement by the model. Thus, it is quite possible that these features in the data are fortuitous.

Using the Fe/O and \(^{22}\)Ne/\(^{20}\)Ne ratios as indicative of the elemental and isotopic enhancements that can be obtained from the model, we carried out a more thorough investigation of the model predictions as a function of grammage and spectral index. The righthand panel of Figure 4 shows contours of constant enhancements of the two ratios as functions of \(\gamma\) versus \(L\). The enhancements of these ratios have significant correlations, particularly for grammages \(<300 \mu g/cm^2\), where the contours of constant Fe/O and \(^{22}\)Ne/\(^{20}\)Ne are approximately parallel. For large values of the grammage, the contours of constant Fe/O become nearly vertical and are no longer parallel to the isotope contours. This suggests that it may be possible to account for the observed enhancements using \(500 \lesssim L \lesssim 800 \mu g/cm^2\) and \(\gamma > 10\). To date, this region of
Figure 4. Left panel: Same as the righthand panel in Fig.3 except with $\gamma = 9.0$. Right panel: Contours of constant enhancement factors for the calculated ratios Fe/O (blue) and $^{22}\text{Ne}/^{20}\text{Ne}$ (red) as a function of grammage ($L$) and spectral index ($\gamma$).

parameter space has not been explored.

4. Enhancement Correlations
Strong correlations have been reported between the event-to-event variations of $^{22}\text{Ne}/^{20}\text{Ne}$ and $^{26}\text{Mg}/^{24}\text{Mg}$ [9] and also between $^{22}\text{Ne}/^{20}\text{Ne}$ and Fe/O [13]. We have investigated whether the model can account for these correlations. The isotope measurements from [9] are shown in the lefthand panel of Figure 5 and are compared with calculated values obtained from the model for a variety of different values of $L$ (distinguished by line color) and $\gamma$ (indicated by points along the lines). The dash-dot line shows the fit to the $^3\text{He}$-rich SEP event data points from [9]. The model does a reasonable job of accounting for the correlation slope between the two isotope ratios, with only a weak dependence on the exact choice of the model parameters. The righthand panel of Figure 5 shows the $^{22}\text{Ne}/^{20}\text{Ne}$ enhancement versus the Fe/O enhancement for $^3\text{He}$-rich events (yellow points) measured with ACE/SIS [13] and for a set of gradual SEP events [14, × symbols]. The slope of the correlation between $^{22}\text{Ne}/^{20}\text{Ne}$ and Fe/O that is predicted by the model is distinctly shallower than observed in the data, but is comparable to the slope found in the gradual events. In addition, as noted above, the largest values of the $^{22}\text{Ne}/^{20}\text{Ne}$ enhancement cannot be obtained using the parameters found by M&K to account for the pattern of elemental abundance enhancements. Further investigation of this correlation in the high-$L$, high-$\gamma$ region of the contour plot in Figure 4 appears warranted.

5. Discussion
Although the model provides some interesting insights into the sort of fractionation effects that can occur when heavy nuclei penetrate a thin H gas layer before undergoing the final step in their acceleration, the model does not include a realistic description of the material that the pre-accelerated particles would encounter in the solar corona where temperatures greatly exceed...
the few $\times 10^4$ K above which H should be fully ionized. M&K discussed the expected effects on the elemental enhancements if the stopping medium is a hot H plasma rather than a neutral H gas. They found that qualitatively similar fractionation can occur as a result of the effective charge states acquired by heavy ions as they slow in the plasma, but with a smaller grammage required and with a $Z$ dependence that is farther from being monotonic. There are significant uncertainties in the calculation of heavy-ion slowing in a hot plasma. In addition to the effects on the effective charge of the energetic ions, the energy loss rate for a given effective charge should be greater than in a gas because energy loss in distant collisions with free electrons can be significantly greater than if the electrons were bound in H atoms [15]. A proper treatment of the fractionation in a hot H plasma is beyond the scope of the present study. Thus the results presented here are, at best, an indication of the types of isotope ratio enhancements that might be expected from a more complete model.

Figure 5. Left panel: Measured Ne and Mg isotope ratios reported in $^3$He-rich SEP events [9] shown as yellow circles with areas inversely proportional to the measurement uncertainty to emphasize the highest-precision measurements. Yellow square shows the average enhancement in a number of $^3$He-rich events too small to include individually. Points indicated by $\times$ are from large, gradual SEP events [14]. Calculated enhancements are shown as diamonds for grammages of 100 (black), 200 (red), 300 (blue), and 400 $\mu$g/cm$^2$ (magenta) and $\gamma=2, 3, \ldots 8$ with the enhancements increasing with increasing $\gamma$. Dash-dot line shows the correlation expected for fractionation proportional to a power of $Q/M$ [16]. Right panel: Correlation between the Ne isotope ratio enhancement and the Fe/O enhancement. Symbols are the same as in the left panel.

6. Summary
We were able to successfully reproduce the M&K calculation of heavy element fractionation resulting from the dependence of specific ionization in a neutral H gas on atomic number and energy per nucleon. Carrying out the calculations using Geant4 and using the same grammage and spectral index of the incident power-law energy spectrum gave enhancements that are quantitatively very similar to those obtained by M&K. We then applied this calculation to investigate isotopic fractionation effects. To account for observed isotope ratio enhancements, we required significantly more extreme power-law spectra than obtained from the elemental
enhancements. A more extensive search of the parameter space of grammage versus spectral index did not establish conditions under which observed enhancements of both Fe/O and $^{22}$Ne/$^{20}$Ne could be obtained simultaneously using a neutral H gas as the stopping medium, but did identify a trend that suggests that further investigation is warranted of the region with $500 \leq L \lesssim 800 \mu g/cm^2$ and $\gamma > 10$. The model did yield correlations between enhancements of different isotope ratios that are similar to those that have been measured, but did not reproduce the more extreme enhancement factors that have been observed. An improved assessment of the model will require an accurate treatment of heavy ion stopping in a hot, fully-ionized plasma.

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