Isotopic composition of Kr in presolar mainstream SiC grains

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Updated neutron capture cross sections of Kr isotopes have been measured by Mutti et al. (2002) with an uncertainty of 5% (1σ). This allows a reanalysis of *s*-process Kr predicted in asymptotic giant branch stars (AGB) and its comparison with meteoritic Kr-S carried by presolar SiC grains (Lewis et al., 1994).

Figs. 1 and 2 compare the Kr-G component calculated from isotopic analyses of aggregates of millions of SiC presolar grains for several grain size separates with theoretical predictions in AGB stars. Fig. 1 shows pure He shell material predicted for solar metallicity $1.5M_{sun}$ AGB stars and Fig. 2 shows the same predicted for half-solar metallicity and $3M_{sun}$. Increased ^{13}C-pocket efficiency raises ^{86}Kr and to a lesser extent, lowers ^{80}Kr and raises ^{84}Kr; the range of efficiencies are shown as shaded bands.

The two cases cover the range of mass and metallicity thought likely for the AGB star sources of presolar SiC. Our preliminary interpretation is that the smaller size grains showing the lowest $^{86}Kr/^{82}Kr$ and the higher $^{80}Kr/^{82}Kr$ are preferentially formed in AGB stars of lower mass and solar metallicity; the coarsest SiC grains are formed in AGB stars of half-solar metallicity, both in $1.5M_{sun}$ (not shown) and in $3M_{sun}$.
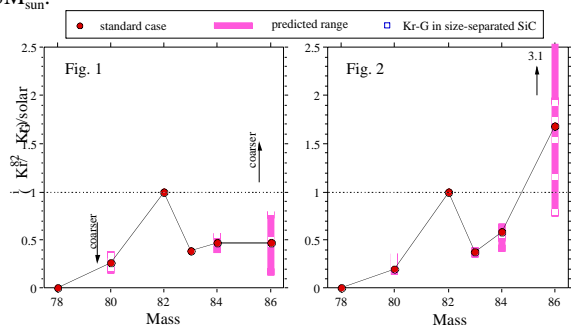
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Deviation from Rayleigh isotope fractionation during Mg evaporation into Mg-containing ambient gas

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In [1], a technique was developed for calculating vapor pressures over completely molten $CaO-MgO-Al_2O_3-SiO_2$ (CMAS) droplets in an ambient gas of any composition using activity-composition models. The vapor pressures were used in the Hertz-Knudsen (HK) equation to compute the effects of ambient gas composition on the chemical and isotopic changes of a liquid having the composition of a refractory nebular condensate during cooling and evaporation in an 11-element closed system of solar composition. These effects are significant when $P_{Mg}^{amb}/P_{Mg}^{vap}=0.1$, where P_{Mg}^{vap} and P_{Mg}^{amb} are the vapor pressure of Mg and its ambient pressure in the gas reservoir, resp. In this system, only ~5% of the Mg is initially in the liquid, and it evaporates as monatomic Mg. Using the HK equation for each Mg isotope, the Mg isotopic composition of the net flux across the droplet-gas interface is:

$$\frac{J_{25}}{J_{24}} = \sqrt{\frac{m_{24}}{m_{25}}} \frac{(X_{25}P_{Mg}^{vap} - Y_{25}P_{Mg}^{amb})}{(X_{24}P_{Mg}^{vap} - Y_{24}P_{Mg}^{amb})}$$

where $J_{25(24)}$ and $m_{25(24)}$ are the net flux and mass, resp., of ^{25}Mg (^{24}Mg), and $X_{25(24)}$ and $Y_{25(24)}$ are the abundances of ^{25}Mg (^{24}Mg) as a fraction of the total Mg in the droplet and in the ambient gas, resp. Results are compared to a reference calculation for vacuum evaporation using the Rayleigh equation in which the gas/liquid distribution coefficient equals the inverse square root of the isotopic masses. During cooling from 1700 to 1500 K at 4 K/hr at $P_H^{tot}=1.67*10^{-2}$ bar, $\delta^{25}Mg$ and $\delta^{26}Mg$ of the liquid rise, reach a maximum and fall further and further below their Rayleigh curves with increasing fraction of ^{24}Mg evaporated, as seen in [2]. This profile is due to isotope exchange with the ambient gas which undergoes complementary changes in chemical and isotopic composition. Progressively greater evaporation causes gradual departure of the slope of $\ln(R/R_o)_{26/24}$ vs. $\ln(R/R_o)_{25/24}$ from the Rayleigh curve, where R and Ro are the Mg isotopic ratio of the liquid; and the initial, normal ratio; resp. After the ratios reach their maxima and begin to decline, the departure reaches its maximum and then falls, ultimately reaching ~0. $\Delta^{25}Mg$, the departure of $\delta^{25}Mg$ from what is expected from Rayleigh fractionation, is computed by multiplying $\delta^{26}Mg$ calculated at any temperature step by the $\delta^{25}Mg$ / $\delta^{26}Mg$ ratio of the Rayleigh fractionation curve at a given $\delta^{25}Mg$, and subtracting the result from $\delta^{25}Mg$ calculated at the same temperature step. In the present case, $\Delta^{25}Mg$ reaches a maximum of ~-1.2 ‰ at 98.6 % of ^{24}Mg evaporated, and then returns to near-zero at ~99.1 % evaporated. Such departures from Rayleigh fractionation could be used in principle to distinguish lightly from heavily evaporated residues that have the same $\delta^{25}Mg$ due to back reaction of the latter.

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