Source of the Rare-Earth Element Peak in r-Process Nucleosynthesis

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(Received 26 December 1996)

We use network calculations of r-process nucleosynthesis to pin down the origin of the peak in the solar r-process abundance distribution near nuclear mass number $A \approx 160$. The peak is due to a subtle interplay of nuclear deformation and β decay, and forms not in the steady phase of the r process, but only just prior to freeze-out, as the free neutrons rapidly disappear. Its existence should therefore help constrain the conditions under which the r process freezes out. [S0031-9007(97)04032-5]

PACS numbers: 26.30.+k

The r process is responsible for synthesizing roughly half the heavy nuclei in the solar system [1]. It is widely believed to occur in type II supernovae, beginning at a time when the density of free neutrons is so high that neutron capture by nuclei occurs much more rapidly than nuclear β decay. Under these conditions equilibrium between neutron capture and photodisintegration [called (n,γ)-(γ,n) equilibrium] establishes itself so that before long very neutron-rich isotopes of each element are populated with their relative abundances set only by their neutron separation energies and partition functions, and the temperature and density of the environment. Towards the end of this "steady" phase of the r process—so called because creation and destruction reactions balance and abundances change slowly—the neutrons begin to disappear, making (n,γ)-(γ,n) equilibrium more difficult to maintain and causing nuclear abundances to change rapidly. Eventually the neutron capture and photodisintegration reactions "freeze out," and the nuclei simply β decay back to the stability line to give the final r-process abundances.

The dominant features in the solar r-process abundance distribution are large peaks at nuclear mass numbers $A \approx 80$, 130, and 195. These form as the nuclear flow passes through neutron-closed-shell nuclei, which capture neutrons reluctantly and have long beta-decay lifetimes, acting as bottlenecks at which abundances build up. This mechanism for peak formation has been well understood for many years [2]. The second most pronounced feature in the abundance distribution is a smaller but still very distinct peak at $A \approx 160$, the region of the rare-earth elements (REEs). In contrast to the major peaks, its origin has remained something of a mystery since its presence was noted in the first detailed compilations of solar-system abundances [3,4]. In this paper we show that the REE peak is due to deformation in nuclei created *after the steady phase of the r process ends*. Previous r-process studies have usually limited themselves to the steady phase. Thus, although deformation has long been suspected to play a role in the formation of the REE peak [2], no compelling connection has been made until now.

Nuclei deform when deformation increases stability. Up to a point, increasingly neutron-rich isotopes of an element can thus gain relative stability by increasing their deformation. At some isotope, however, deformation can increase no more; the next isotope is then less stable. Because of the sudden drop in binding energy with the addition of a neutron a deformation maximum can mimic a closed neutron shell. In the early scenario of Ref. [2], the deformation maximum is encountered near $A = 160$ during the steady phase of the r process, with the drop in binding energy after the maximum leading to a smaller version of the peaks at $A = 80$, 130, and 195. Although this hypothesis was initially plausible, it began to suffer when nuclear masses far from stability were understood well enough to carry out real calculations. The work of Ref. [5], for example, did produce an abundance hump in the REE region, but one that was much broader than the observed peak. In addition, the conditions required by the mechanism of Ref. [2] made other r-process features more difficult to reproduce. A second explanation, first proposed in Ref. [6] and elaborated on in Ref. [7], is that the REE peak is produced by mass-asymmetric fission of very heavy r-process nuclei. For a number of reasons, however, this idea is no longer compelling either [8].

Despite the lack of a good explanation, recent r-process simulations [9,10] in the high-entropy neutrino-driven bubble near the surface of a nascent neutron star produced a realistic REE peak. The simulations used calculated nuclear properties (far from stability) in which the effects of deformation had been included self-consistently. Furthermore, they were among the first to follow the r process all the way through freeze-out and did not allow nuclear fission. The success of these full-blown supernova simulations in forming an REE peak, not explained in Refs. [9,10], points to the poststeady phase of the r process and motivates the simpler calculations described below that get at the cause of the peak.

A crucial concept for our analysis is the r-process "path" through the N-Z plane, which we define as follows: At any given time, for each element with proton number Z, there is an isotope with maximum abundance; the collection of all such isotopes defines the path at that time. As long as β-decay rates are much less than neutron-capture or disintegration rates and the system is in (n,γ)-(γ,n) equilibrium, the path's location follows from the requirement that the average free energy be stationary under the transfer of a neutron from a nucleus to the free-neutron bath. This in turn means roughly that for every Z the isotope with maximum abundance has a neutron separation of

$$S_n(Z,N_{\max}) = -kT\ln\left\{\frac{\rho N_A Y_n}{2}\left(\frac{2\pi\hbar^2}{m_n kT}\right)^{3/2}\right\}, \quad (1)$$

where $N_{\max}$ is the neutron number of the isotope, T is the temperature, ρ is the mass density, N_A is Avagadro's number, Y_n is the abundance of free neutrons per nucleon, and m_n is the neutron's mass. Equation (1) shows that for given T, ρ, and Y_n, the equilibrium path always lies along a contour of constant separation energy.

The high-entropy r-process calculations of Refs. [9,10] alluded to above were performed within the context of detailed supernova simulations. To get a clear picture of the dynamics of the r-process path, here we simply parametrize the dependence of temperature on time (with $\rho \propto T^3$ and assuming a simple constant outflow velocity [11]) to roughly match the results of the more complicated calculations. We then solve the network differential equations (described in Ref. [1]) that determine the time development of nucleosynthesis. The inputs, besides the temperature and density, are the initial mass fractions of neutrons and preexisting "seed" nuclei, and calculated neutron capture rates [1], neutron separation energies [12], and β-decay rates [12]. The seed nuclei quickly come into (n,γ)-(γ,n) equilibrium and then undergo the usual β-decay and neutron-capture sequence. We run the simulations through freeze-out until only stable nuclei remain. The treatment is fully dynamical in that neutron capture and photodisintegration continue to compete with β decay throughout the entire process, even when equilibrium no longer obtains. In the more detailed supernova simulations, the high-entropy r process occurs over several seconds, and many r-process components combine to give the final abundance distribution (see, e.g., Fig. 15 of Ref. [10]). The calculations presented here treat just the components with the highest initial neutron/seed nucleus ratios, because they are responsible for the REE peak. These components are also responsible for the large peak at $A \approx 195$ in the more detailed simulations. In fact, no matter what the precise conditions in the supernova, virtually any high-entropy r-process component that produces the $A = 195$ peak with sufficient abundance and in the correct location also makes a REE peak [11] if freeze-out is treated dynamically.

A sample set of r-process abundances resulting from our calculations appear in Fig. 1(a) alongside the measured solar-system abundances. In this run the initial seed nucleus was ^{70}Fe and the initial value of R, the ratio

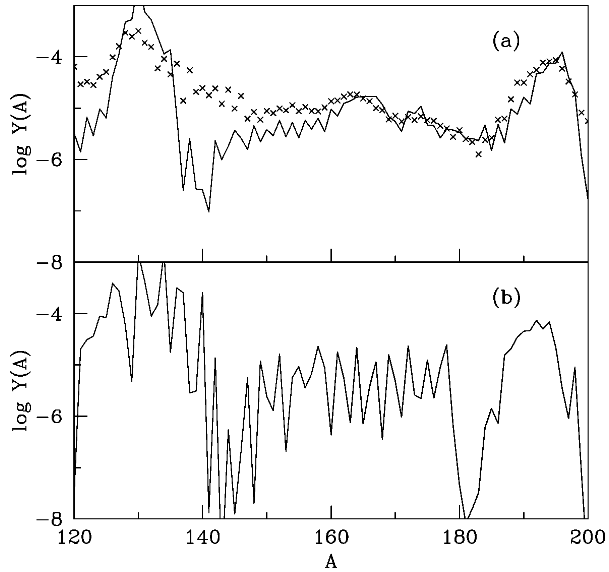

FIG. 1. Calculated (line) and measured (crosses) solar r-process abundances. (a) shows the final calculated abundances and (b) the calculated abundances before freeze-out, while the r process is in the steady phase.

of the abundance of free nucleons to that of nuclei was 57, implying that a seed captured on average 57 neutrons over the duration of the r process. The trough in the calculations just above the peak at $N \approx 82$ ($A \approx 130$) can be largely filled in by another component with slightly different temperature and neutron density. What is important is the presence of a REE peak at approximately the correct location and with the correct width. No sign of this peak exists during the steady phase of the r process [Fig. 1(b)]. It forms only after R falls below about 1, when steady β flow is destroyed and the path begins to move towards stability. The peak appears under a wide range of initial temperatures, densities, and neutron/seed ratios, as well as changes by factors of 5 or more in all calculated β-decay rates, provided only that freeze-out is prompted by the capture of nearly all free neutrons rather than a sudden drop in overall density and temperature, as is sometimes assumed. The primary reason, surprisingly, is that if the temperature and density do not change precipitously the r process stays in approximate (n,γ)-(γ,n) equilibrium even after steady flow fails. Only when R has fallen by many orders of magnitude does β decay completely dominate the other reactions and destroy the remnants of (n,γ)-(γ,n) equilibrium. As a result, the path continues for some time to lie roughly along contours of constant neutron separation energy as it moves towards stability. It is during this time that the REE peak forms.

Figure 2 illustrates the persistence of approximate (n,γ)-(γ,n) equilibrium; it shows the path between $N = 82$ and 126 at three times during a 0.25-sec interval just after the steady phase ends. During this period, as indicated by the inset of Fig. 2, R (or Y_n) drops dramatically (the diamonds mark the three times at which the

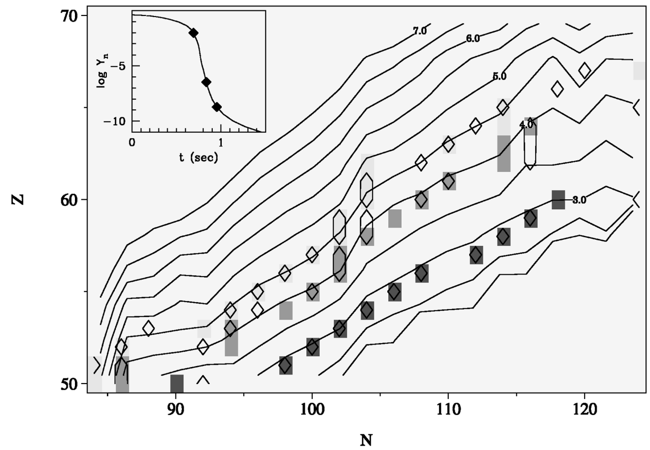

FIG. 2. The r-process path between $N = 82$ and 126 at three times during a 0.25-sec interval early in the decay to stability. The shaded squares are the actual paths, the lightest corresponding to the latest time, and the diamonds the equilibrium paths defined at the same times by Eq. (1). The lines are contours of constant separation energy in MeV. The inset shows the neutron abundance per nucleon over this interval, with the three times at which the path is depicted indicated by diamonds.

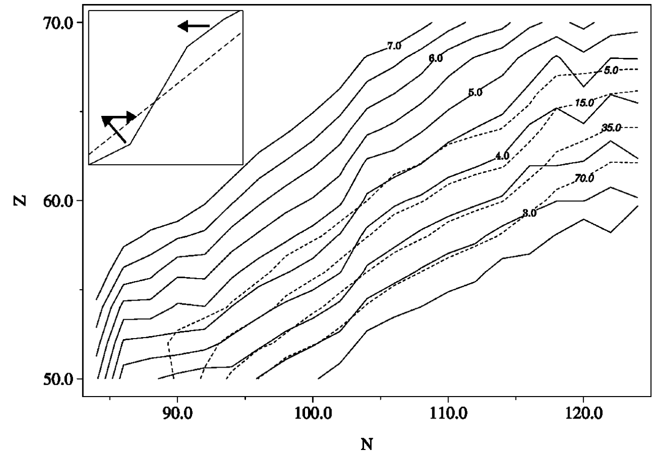

FIG. 3. Contours of constant neutron separation energy in MeV (solid lines) and constant β-decay rates in s^{-1} (dashed lines). The inset is a schematic of two such contours, with the arrows depicting the flow of nuclei into the region containing the separation-energy kink.

path is plotted), while T and ρ change slowly, with the net result according to Eq. (1) that the path moves back towards more stable nuclei with higher neutron separation energies. The dark squares in the large figure are the paths as defined above, with the upper set corresponding to the later time. The open diamonds indicate the "equilibrium paths," i.e., those that would obtain if the system were in true (n, γ)-(γ, n) equilibrium according to Eq. (1). Contours of constant neutron separation energy for the even N nuclei are overlaid. The actual and equilibrium paths indeed differ very little well after the end of the steady phase. Eventually (and importantly), as the figure shows, a "kink" in the separation energies at $N \approx 104$ is intercepted and imposes itself on the path.

Large kinks in the path are the underlying cause of the abundance peaks at the neutron closed shells mentioned above. Because the neutrons in all these nuclei are strongly bound the path turns sharply up towards stability when a closed shell is reached, producing a concentration of populated isotopes close together in A with relatively long β-decay lifetimes. The early steady-phase explanation of the REE peak in Ref. [2] is a variation on the same theme. In our simulations, however, the REE peak does not form in exactly this way, even though it is clearly associated with the $N \approx 104$ kink, which in turn is clearly due [12] to the deformation maximum postulated in Ref. [2]. The nuclei at the top of the kink, and thus closer to stability, do have moderately slower β-decay rates than those along the path immediately below, but neither this fact nor the proximity of the kink nuclei to one another along the path account entirely for the pronounced REE peak. Another mechanism, relying on the motion of the path towards stability after the failure of steady flow, is also at work.

Once steady flow ceases, Y_n falls rapidly compared to the rate of decline in temperature and density. By Eq. (1) then, the path moves quickly towards stability at a rate governed by the average β-decay lifetime for nuclei lying on the path. During the interval when the path runs through the kink, this average rate is typically the rate of a nucleus in the kink itself. Below the kink, as illustrated in the center of Fig. 3, the nuclei along the path are farther from stability and therefore decay faster than average, i.e., before the average separation energy has changed enough to move the equilibrium path in their vicinity. In an attempt to return to the path and stay in equilibrium, these nuclei then capture neutrons, increasing their value of A. The nuclei above the kink, by contrast, decay more slowly than average, and in general will not do so before the equilibrium path at their location has moved. When it does move, these nuclei, whose thermodynamic impetus is also to remain in equilibrium at the average separation energy, photodisintegrate so that their mass number A is lowered. In fact, it is these disintegrating nuclei above the kink that supply in part the neutrons for capture by β-decaying nuclei below the kink. The net result, shown with arrows in the inset in Fig. 3, is a funneling of nuclei into the kink region as the path moves toward stability.

To show that this mechanism is both simple and robust, we ran a simulation with our own simplified and easily varied nuclear properties. We obtained binding energies from a simple semiempirical mass formula ([13]) and β-decay lifetimes by fitting those of Ref. [12] with a function of the form $T_{1/2} = aQ^{\alpha}$, where Q is the difference in binding energies between the parent and daughter and the best fit was obtained with $a = 250$ and $\alpha = -3.80$. We assumed neutron capture rates, the details of which are irrelevant, to have an exponential dependence on separation energy, reflecting their dependence on the level density in the compound nucleus formed by capture. We started the simulation at the end of the steady phase of

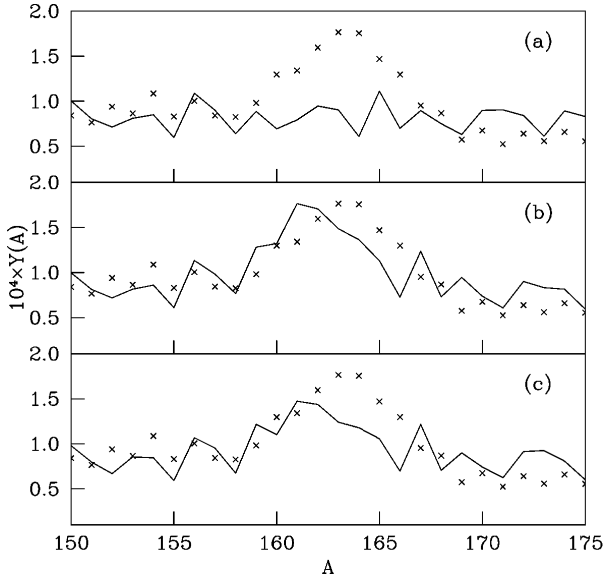

FIG. 4. Abundances on a linear scale near $A = 160$ in the simplified model (see text). (a) is with smooth separation-energy contours, (b) with a kink in the contours, and (c) with constant β-decay rates along each kinked contour. The crosses are the appropriately scaled solar abundances.

the r process, with abundances along the equilibrium path between $N = 82$ and $N = 126$ taken to be identically normalized Gaussian curves of width 1.05 centered for each Z at the values of $N_{\max}$ produced by our more realistic model. These conditions produced a flat final abundance curve, shown in Fig. 4(a) alongside the (appropriately scaled) solar abundances. When we introduced a kink into the separation energies at $N = 104$, adjusting the capture and β-decay rates to reflect the new bindings, a REE peak matching that in the solar-abundance curve formed [Fig. 4(b)]. But when we modified the β-decay rates to be constant along curves of constant separation energy, destroying the β-decay-induced dynamic described above, the peak shrank by a factor of about 2 relative to the surrounding abundance level [Fig. 4(c)]. This smaller peak therefore represents the effects of the concentration of points along the path and the slight increase in β-decay lifetimes at the top of the kink. These factors alone are clearly not enough to produce the entire REE peak. If, among other possibilities, the steady r-process path runs through the kink, as postulated in Ref. [2], the peak will not fully form. We conclude that although this peak is indeed due to a deformation maximum in the region, it forms only *after* the steady phase of the r process ends.

If our argument is correct, the existence of the peak has important consequences both for the supernova nucleosynthesis and for the nuclear physics of neutron-rich nuclei. First, it means that the r-process path must be moving back towards stability when freeze-out occurs. This can happen only if freeze-out is prompted by the exhaustion of free neutrons. If the freeze-out of a high-entropy ($\rho \propto T^3$) r process is instead prompted by a rapid drop in the temperature, the path will always move away from stability towards nuclei with very low neutron separation energy, and no REE peak will form. This fact argues against models in which the expansion of the r-process region is so fast that freeze-out occurs before the neutrons have all been captured. Second, regarding nuclear structure, the peak confirms the predicted deformation of neutron-rich rare-earth nuclei. We expect future work on formation of the REE peak to yield other important insights.

The authors are grateful to D. H. Hartmann and D. D. Clayton for discussions. This work was supported by the U.S. Department of Energy under Grant No. DE-FG05-94ER40827 and by NASA under Grant No. NAGW-3480. We thank the Institute for Nuclear Theory at the University of Washington, where some of this work was carried out.

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