Electron Screening in Metals

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Electron screening significantly enhances cross sections for reactions between charged nuclei at astrophysically relevant energies. Until now the process of screening has been treated by a static decrease of the Coulomb barrier due to the presence of electrons. It was shown many times, including the work described below, that such theoretical approaches cannot explain the measured electron screening potentials, especially in the case of metals, where values way above all theoretical limits have been deduced. Moreover, by measuring electron density with proton NMR we showed that a large static increase of electron density is unrealistic in solid state. Instead, we suggest a novel dynamic approach to electron screening where both approaching nuclei are dressed with electrons. In the studied p+Ni reaction the projectile electron is treated quantum mechanically, the wave function evolving in time dependent potential generated by both nuclei.

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1. Introduction

The nuclear reaction cross section *σ(E)* is in nuclear astrophysics often written as a function of c.m.s. energy E as

$$\sigma(E) = \frac{S(E)}{E} e^{-2\pi\eta},$$

where S is the astrophysical S-factor, $\eta = Z_1 Z_2 e^2 / 4\pi\varepsilon_0 \hbar \sqrt{(2E/\mu)}$ the Sommerfeld parameter, Z_1 and Z_2 the charge numbers of interacting nuclei and μ their reduced mass. The Gamow factor $e^{-2\pi\eta}$ approximately describes the Coulomb barrier penetrability. Electron screening enhances cross sections for reactions between nuclei at low energies and the enhancement factor *f* can be defined as *f(E)=σ(E+U_e)/σ(E)*, where U_e is the screening potential [1]. The magnitude of the screening potential can be estimated from the adiabatic limit that defines the maximum energy available for screening from the difference in atomic binding energies of the reactants and reaction products. Indeed, for all gaseous and insulating targets the measured screening potential was close to the adiabatic limit. On the other hand, for a large number of metallic targets screening potentials an order of magnitude larger than the adiabatic limit were measured [2-6]. The reason for such discrepancy is presently not understood. An approach using the Drude-Debye model has been proposed [2], but electron densities an order of magnitude higher than are known to exist in solid state were required to explain the measured screening potentials in metallic targets. We will present below a novel approach to electron screening that may show us a possible way forward in our understanding of the problem.

2. The palladium hydrogen system

First we studied the ^{1}H(^{7}Li,α)^{4}He reaction in inverse kinematics as described in ref. [7]. Contrary to all previous experiments, where hydrogen was forced into metals using ion beam implantation, in our case it was loaded into Pd and PdAg alloys from gas phase. We observed large electron screening only when the metallic targets were under mechanical stress, while without stress the potential was consistent with the adiabatic limit. Contrary to previous suggestions we have shown that the screening potential does not depend on the Hall coefficient of the metal [2] nor on hydrogen concentration in the metal [3]. It is known in some crystals (V, Nb, Ta) that under mechanical stress hydrogen moves from its original tetrahedral positions to dislocated tetrahedral position in the bcc crystal lattice [8]. We believe something similar happens in the PdH system. Hydrogen probably moves from octahedral to dislocated octahedral positions in the fcc Pd lattice. To substantiate this claim we measured the Knight's shift with ^{1}H nuclear magnetic resonance (NMR) technique [9]. Namely, the Knight's shift originates from the interaction of conducting electrons in metals with nuclear spins and is proportional to the average probability density at the nucleus site for all electronic states at the Fermi surface.

The ^{1}H NMR lineshapes were measured at 2.35 T (equivalent to 100 MHz proton frequency). A 47μm thick 2.5x2.5 cm PdH foil with initial H/Pd concentration of 0.7 was inserted in the rf coil and two sides were fixed to a stretcher. The stretcher was made of non-metallic material (fiberglass). The Hahn echo pulse sequence (π/2-τ-π-echo) was used with the

π/2 rf pulse length of 8 μs and the inter-echo time τ of 70 μs. The [1]H Hahn echoes were measured before and after the foil was exposed to mechanical stress, i.e. the foil was stretched with a pressure of about 220 MPa. The stretching pressure is relatively small but it similar to the pressures used in our electron screening work [7]. The [1]H Knight's shifts were measured with respect to the position of the stretcher signal that is clearly visible in the spectrum (Fig. 1). The position of the stretcher signal is almost indistinguishable from water signal that is often used as a reference. To be able to obtain the real proton Knight's shift K_H without the contribution of the demagnetizing field, which is due to the overall macroscopic sample shape, the experiments were performed with foil parallel and perpendicular to the applied static magnetic field. Assuming that our foil can be approximated by the infinite sheet and the fact that the symmetry of the electron environment of the ^{1}H spins is cubic, the true Knight's shift is given by [10, 11]

$$K_H = S(0°) - \frac{4\pi}{3}\chi_V - \sigma \ ,$$

where $S(0°)$ is the shift at parallel position with respect to static magnetic field B_0, χ_V the bulk susceptibility of the sample that can be expressed as $\chi_V = \left[S(0°) - S(90°) \right]/4\pi$ and σ is the frequency of the non-metallic reference material, i.e. the stretcher protons in our case.
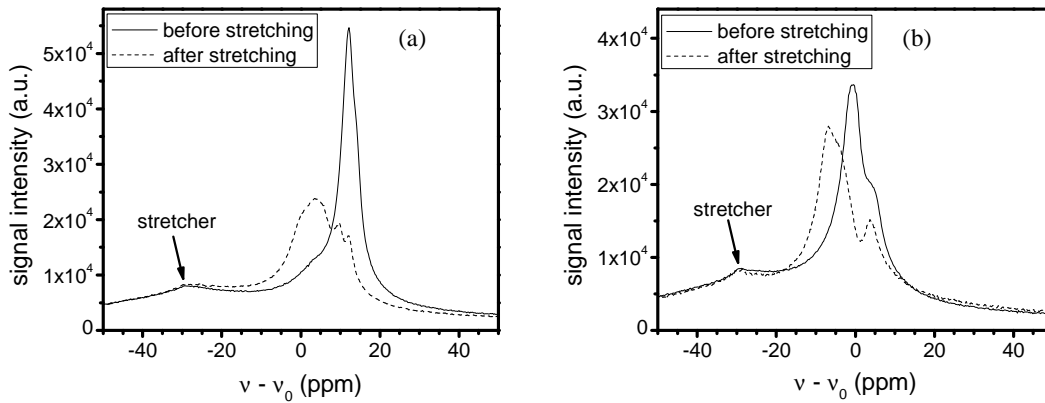

Fig. 1: ^{1}H NMR lineshapes in (a) perpendicular and (b) parallel orientation with respect to B_0.

It can be seen from fig. 1 that before application of mechanical stress a single line with a small bump was observed in both orientations. The reason for the bumps is that the foil was not completely flat and therefore some parts of the foil were not parallel or perpendicular to the external magnetic field. The shift of 32.8 ± 0.2 ppm was measured relative to the signal of the stretcher. After the foil was stretched the single ^{1}H line splits into three lines and the shifts of 25.9 ppm, 29.4 ppm and 35.8 ppm were determined after stretching. It is known that the Knight's shift in PdH$_x$ system strongly depends on H concentration [12, 13] and that the H concentration decreases with time. To determine the relative shift that originates from lower H concentration we also measured time dependence of the Knight's shifts of the PdH foil without mechanical stress. In this case the ^{1}H line shifted to lower frequencies, but no splitting was observed. In this latter measurement the Knight's shift of 33.2 ppm was measured at H

concentration of 0.7 and after 40 minutes (the same time as for the measurements with mechanical stress) the shift was 31.1 ppm. Therefore the shift of $\approx$-2 ppm was attributed to changes in H concentration in the PdH foil. Consequently the nuclei with the Knight's shift of 29.4 ppm were assigned to the position which did not change under mechanical stress, and the nuclei with the Knight's shifts of 25.9 ppm and 35.8 ppm to the nuclei that moved to positions with lower and higher electron densities, respectively. This implies a static electron density change of at most 20% compared to non-stretched PdH foils, where no large electron screening was observed. As stated above some hydrogen stays in its original position and under stress does not move to a position where high electron screening was measured. This probably explains why we measured almost a factor of 2 lower electron screening potential compared to ref. [4].

An analogous trapping of hydrogen has been extensively studied after ion beam implantation into various metals [8]. In this case hydrogen is trapped to crystal defects (vacancies or radiation damage) caused by beam implantation. Again hydrogen moves from its original position towards the vacancy in the crystal where the electron density is different. The different ability of various metals to trap hydrogen to crystal defects may actually be the cause of very large differences in measured electron screening potentials [2]. For example, Pd has one of the highest U_e values but also a very low solubility of hydrogen, which probably means that the majority of hydrogen in Pd is trapped. When the same system was measured at higher hydrogen concentration, a lower U_e value was obtained [3]. This suggests that the measured U_e is actually weighted by the ratio of trapped vs. not trapped hydrogen.

3. High Z screening

It has been observed in reactions between protons and Li, Be, V and Lu that electron screening is roughly proportional to the Z of the target [4,5]. Particularly interesting was a measured shift in proton energy at which a resonance in the ^{176}Lu(p,n)^{176}Hf reaction was detected in metallic compared to insulating environment [5]. No plausible explanation was given for this observation and it is by itself difficult to accept, since it implies a binding energy change of the ^{176}Hf nuclear reaction product. To better understand this strange observation we checked for energy shifts in the ^{58}Ni(p,γ) and ^{58}Ni(p,p'γ) reactions that have a number of sharp and easy-to-detect resonances [14]. We observed no shifts in ^{59}Cu resonance energies in metallic Ni compared to insulating NiO targets. On the other hand, we observed different resonance strengths in different environments. These differences could be attributed to electron screening. However, the analisys of different resonances and even of different γ rays from the same resonance did not give a unique electron screening potential. The most reliable result was obtained from the ^{64}Ni(p,nγ) ^{64}Cu reaction. By comparing thick target γ-ray yields from Ni and NiO targets and by properly taking into account different stoichiometries and stopping powers in these two materials we obtained an electron screening potential of about 31 keV. This value is close to both V and Lu screening potentials [5], as expected, but again an order of magnitude above the adiabatic limit.

Large electron screening in metals was explained using a Debye plasma model applied to valence electrons [2]. However, the proposed model has a few pitfalls, when used for a metal.

The electron Debye length around the nickel nuclei in the lattice is about one tenth of the Bohr radius. This implies that valence electrons in Ni cluster in a sphere with a radius *r* of a few K shell radii, which is physically impossible. Electron density around a nucleus obtained by using Debye model is given by equation:

$$\rho_e(r) = -\frac{Ze}{4\pi r}\kappa^2 e^{-\kappa r},$$

where κ is inverse of the Debye length and Z the charge number of the target nucleus. By integrating the above equation in a sphere with a radius equal to the Bohr radius we find that the number of electrons in this volume is equal to Z. In the case of Ni that would mean that all electrons (both free and bound) are concentrated in a sphere with a radius approximately equal to one third of the radius of the whole atom, which is again physically impossible. In spite of giving a good parametrization to the data, the Debye plasma model is evidently unsuitable for describing electron screening in metals. Hence, we tried a different approach to the problem. Instead of assuming that electrons in the crystal tend to cluster around the nucleus in the same manner as in plasma, we used quantum mechanical approach. We treated valence electrons as the s-waves scattered by a Coulomb potential of the target nucleus. (The s-wave approximation is justified at electron energy of 1/40 eV). The s-wave component of the partial-wave expansion of Coulomb wave function is equal to [15]:

$$\psi_e = \frac{1}{L^{3/2}}\frac{1}{kr}e^{i\delta_0}F_0,$$

where *k* is a wave vector, the wave function is normalized within a cubic box of side L, δ_0 is a Coulomb phase shift, and F_0 solution to the radial Schrödinger equation in the Coulomb potential of a point nucleus [15]:

$$\left(\frac{d^2}{dr^2} - \frac{2\eta k}{r} + k^2\right)F_0(kr) = 0.$$

Taking into account that $F_0 = C_o(\eta)kr\phi_0(\eta,kr)$ and $C_0^2 = \frac{2\pi\eta}{e^{2\pi\eta}-1} \approx 2\pi\eta$ (η~-23 is the Sommerfeld parameter in case of electron scattering on nickel where $Z_1e= -e$, $Z_2e= 28e$) we obtain for the electron probability density:

$$N|\psi_e|^2 = 2\pi\eta|\phi_0|^2 n_e,$$

where n_e is valence electron density. We found ϕ_0 by numerically solving the above Schrödinger equation since no tables of F_0 are available for these extreme *η* values. Assuming that there is one free electron per nickel atom, we obtain that the number of electrons contained in a sphere of radius equal to the Bohr radius is of the order of 0.1. This more appropriate treatment of contribution of valence electrons to electron screening potential obviously cannot produce an order of magnitude higher electron densities than are normal in atoms, as demonstrated in ref. [2] using the Debye plasma model and a static treatment of electrons. We therefore propose a new approach to electron screening that may produce high electron densities required to explain observed large electron screening potentials. Contrary to previous calculations [16], we assumed that both the projectile (proton) and target (Ni) are neutral when approaching each other. Proton

is considered to get dressed via charge exchange effect, while traversing the medium. We treated the nuclei as classical particles and modeled their motion according to Newton's laws. Target electrons are also treated classically, as a uniformly charged sphere of radius equal to atomic radius of the target nucleus. However, the projectile electron is treated quantum mechanically, the wave function evolving in time dependent potential generated by the Ni atom and proton nucleus. By treating projectile electron in this way we expect large increase in electron density at the place of proton at small internuclear distances. Our preliminary results show that electron screening is a dynamic process that can in no way be explained by a static reduction of the Coulomb barrier, neither in solid state nor in plasma.

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