Importance of Polarization of Bound Projectile *s* Electrons for Transient Magnetic Fields

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(Received 22 November 1978)

K-vacancy fractions have been measured for Si ions moving in nickel at velocities between $3.9v_0$ and $9.0v_0$. The observed fractions, 2–23%, provide strong evidence that transient magnetic fields for ions moving in magnetized materials are caused mainly by bound, polarized electrons. A polarization close to 0.13 suffices to explain measured transient fields, and it is argued that the polarization can be due to a combination of spin-exchange interactions and capture-loss processes.

Since the discovery[1] of transient magnetic fields acting on swift nuclei slowing down in ferromagnetic materials, a large amount of experimental data has been accumulated.[2] The only existing self-contained theory was proposed by Lindhard and Winther (LW),[3] according to which the transient field is caused by the enhancement of the polarized-electron density occurring at the nucleus because of Coulomb scattering of the continuum electrons on the moving positive ion. Of late, however, it has become clear that the transient field *increases* with increasing ion velocity, in contrast to the LW theory, which predicts a *decrease*.

Eberhardt *et al.*[4] have suggested an empirical expression that reproduces transient-field data remarkably well for ions slowing down in magnetized iron:

$$B(v)=aZRv/v_0, \tag{1}$$

where v is the ion velocity, $R=1+(Z/84)^{5/2}$, and $v_0=c/137$. When this is fitted to experimental observations, the parameter a is found[5] to be independent of Z, $a\sim 110$ kG for ions in the range $12 \leq Z \leq 80$, while large fluctuations are seen for lighter ions.[6] For C ions,[7] the transient field is observed to decrease at velocities larger than $(4 \text{ to } 5)v_0$.

The extremely strong transient fields at high ion velocities are considered to be caused by polarized electrons in *bound* states of the moving ion, as originally suggested by Borchers *et al.*[1] One can express[4] the transient field as

$$B(v)=\textstyle\sum_n \xi^{ns}(v)F_1^{ns}(v)B_{ns}, \tag{2}$$

where $F_1^{ns}(v)$ is the fraction of ions carrying an unpaired ns electron and $\xi^{ns}(v)$ is the degree of polarization of the latter. The magnetic contact field B_{ns} on the nucleus from a single ns electron depends weakly on velocity through the change in screening due to inner and outer electrons. As the polarization of the *orbitals* is expected to be small, the hyperfine interaction will be negligible for all but s electrons. The polarized electrons are assumed to be replaced so frequently that the direction of the transient field can be regarded as fixed in the direction of the external field. This is justified by the present measurements.

The quantity B_{ns} can be quite reliably calculated, but neither ξ^{ns} nor F_1^{ns} is known at present. One should note that F_1^{ns} refers to the ion state *inside* the solid and thus cannot be related directly to charge-state distributions measured *after* emergence from solid foils. Hence experiments have been initiated to measure single-1s-electron fractions F_1^{1s} for light ions moving in solids with special emphasis on iron. The present Letter reports on measurements performed for Si ions moving in nickel (selected for experimental reasons) in velocity range $3.9 \leq v/v_0 \leq 9.0$. In the discussion of transient fields, measured vacancy fractions for Si in nickel were assumed to be comparable to those for Si in iron.

Beams of 10–56-MeV ^{28}Si ions were obtained from the University of Aarhus's model EN tandem Van de Graaf. The analyzed beam was passed through a 5-μg/cm^2 thick carbon foil, and pure charge states from 8^+ to 14^+ were subsequently selected by the switching magnet. Target x-ray yields were measured by a Si(Li) detector positioned at 90° to the beam axis. The normalization was accomplished to within 5% by charge collection on the chamber. Target thicknesses were measured separately by ^{4}He backscattering.

Two experimental methods (I and II, similar to those described in Refs. 8 and 9, respectively) were used. For Si velocities in the range from $3.9v_0$ to $7.2v_0$, method I was used. Targets consisted of self-supporting, 40–100-μg/cm^2 thick nickel foils covered on one side with a very thin (1–2 μg/cm^2) titanium probe layer, the x-ray yield of which is very sensitive to the presence of 1s vacancies in the beam. The Ti K-x-ray production cross section is enhanced by a factor

α for projectiles with one K vacancy compared to projectiles with no K vacancies. Thus with α known, the fraction $F_1^{1s}(T)$ of the beam carrying a 1s vacancy after penetration of a given thickness T of nickel could be deduced from a comparison of the Ti K-x-ray yields in the two cases where either the titanium or the nickel was facing the beam.[8] Corrections were applied for the decrease in yield due to slowing down in nickel.

Values of α in the velocity range from $5.4v_0$ to $9.0v_0$ (Fig. 1) were determined by extrapolation to vanishing titanium thickness in a separate experiment with Si^{11+} and Si^{13+} ions impinging on carbon-backed 1-20-μg/cm^2 thick titanium targets. The solid curve in Fig. 1 was chosen to extrapolate α to the velocities $4.7v_0$ and $3.9v_0$ to an estimated accuracy of 15% and 20%, respectively.

At the velocities $6.2v_0$ and $7.2v_0$, incident beams of Si^{11+} and Si^{13+} were used. From a simultaneous least-squares fit of the rate equation to measured vacancy fractions as a function of thickness T, the equilibrium vacancy fraction $F_1^{1s}(\infty)$ and the cross sections for creation σ_{01} and quenching σ_{10} of 1s vacancies were obtained (Table I). At velocities less than $6.2v_0$, beams with no initial K vacancies were used; hence only values of $F_1^{1s}(\infty)$ could be deduced.

In the second method (II), used for incident Si^{11+}, Si^{13+}, and Si^{14+} at velocities $7.2v_0$ and $9.0v_0$, the nickel itself acts as a monitor of Si 1s vacancies. Targets consisted of nickel foils ranging in thickness from 1 μg/cm^2 to 100 μg/cm^2, the thinner of which were evaporated onto 10-μg/cm^2 carbon backings. The method of analysis is similar to that of Gardner *et al.*[9] except that the energy dependence of the target x-ray-production cross section is taken into account. The results are listed in Table I and are in perfect agreement with those of method I ($v = 7.2v_0$). It should be noted that because of large correlations between the six cross sections involved, definite results can be obtained only by making the reasonable assumption that the equilibrium fraction of double vacancies is negligible at these rather low velocities.

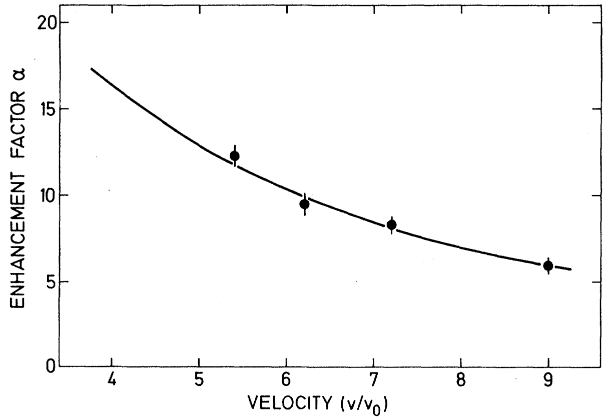

FIG. 1. Measured enhancement factors α at vanishing target thickness for Si ions incident on Ti. The solid curve is a second-order polynomial fit to experimental data.

The single-1s-vacancy fractions obtained for Si in nickel are shown in Fig. 2 (right-hand ordinate). Also shown is the empirical expression (1) for the transient field (left-hand ordinate) with[4] $a = 125$ kG. This should be regarded as representating only the gross features of the velocity dependence.

Measured vacancy fractions were related to transient-field strength with Eq. (2). A value of $\xi^{1s} = 0.13$ was chosen to provide agreement with the empirical expression at high velocities, using a value of $B_{1s} = 460$ MG for hydrogenic Si. However, at lower velocities, single 2s electrons contribute to the transient field. Setting $\xi^{2s} = 0.13$ and $B_{2s} = 50$ MG, we obtain an estimate indicated in Fig. 2, assuming that F_1^{2s} reaches a maximum of 0.5 around a velocity of $v = 4v_0$, corresponding to the orbital velocity of Si 2s electrons. At still lower velocities, a contribution from continuum electrons has been included according to the LW theory.

As seen from Fig. 2, the various contributions, when added, reproduce nicely the velocity dependence of the transient magnetic field observed for Si in iron. This strongly supports the idea that transient fields are mainly caused by *bound* polarized electrons.[1] Furthermore, it is ob-

TABLE I. Measured 1s-vacancy fractions and rearrangement cross sections for Si and Ni.

v/v_0	$F_1^{1s}(\infty)$ (%)	σ_{01} (10^{-18} cm^2)	σ_{10} (10^{-18} cm^2)
3.9[a]	2.3±1.1		
4.7[a]	5.3±1.4		
5.4[a]	8.8±1.0		
6.2[a]	14.9±0.8	0.53±0.08	3.0±0.4
7.2[a]	20.8±0.7	0.79±0.07	3.0±0.3
7.2[b]	20.9±2.9	0.86±0.16	3.2±0.5
9.0[b]	22.6±2.6	1.20±0.20	4.1±0.6

[a] Method I. [b] Method II.

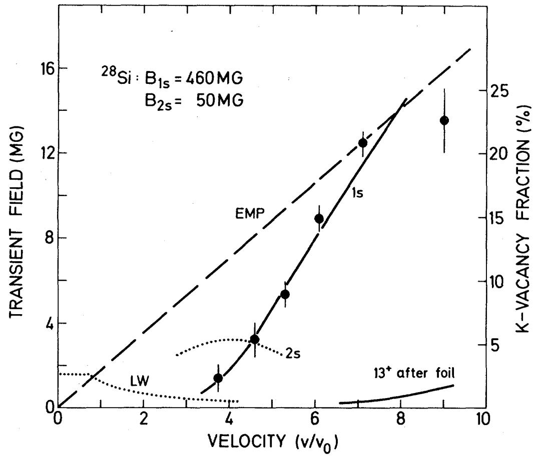

FIG. 2. Measured equilibrium K-vacancy fractions (right-hand ordinate) for Si in Ni with a solid curve to guide the eye. The results are converted into transient-field strength (in Fe) for $\xi^{1s}=0.13$, $B_{1s}=460$ MG (left-hand ordinate). Contributions to the transient field from $2s$ electrons ($2s$) and from continuum electrons (LW) are estimated. The empirical expression (1) for the transient field on Si in Fe is shown as a dashed line. Measured 13$^+$ charge-state fractions are shown (right-hand ordinate) for Si emerging from thin C foils.

served that the degree of polarization for unpaired $1s$ electrons is close to the chosen value of $\xi^{1s}=0.13$, corresponding to the degree of polarization of the Fe M and N shells. According to a Brinkman-Kramers calculation,[10] direct electron capture into the Si K shell will proceed mainly from the Fe L shell and hence cannot explain a degree of polarization of 0.13 (Ref. 4).

We suggest that the transient field arises as a result of two more or less independent processes. First, electron-loss processes produce $1s$ vacancies having little or no polarization, and the lifetime of the vacancies is found from the measured cross sections to be 1–3 fs. Second, the unpaired electrons are polarized through exchange interactions with polarized electrons in higher shells of the ion which, in turn, are polarized by capture-loss and spin-flip[11] collisions with polarized Fe M and N electrons. Comparisons with stopping-power data and measured charge-state distributions show that Si ions do carry several electrons in excited states, and the strong interactions with Fe M and N electrons will ensure that the degree of polarization is close to the average polarization, 0.13, of those. From known atomic energy levels, it can be estimated that the period for the exchange interaction between $1s$ electrons and $2s$, $2p$, and $3s$ electrons of Si is shorter than the measured $1s$-vacancy lifetimes. Thus the transfer of polarization to the unpaired $1s$-vacancy lifetimes. Thus the transfer of polarization to the unpaired $1s$ electron is expected to be almost complete.

In conclusion, the mechanism described will provide a degree of polarization close to 0.13 for all unpaired electrons in ions moving through magnetized iron; still, at high velocities, the figure may become smaller due to the depopulation of the outer shells. Thus, in general, the velocity dependence of the transient field is mainly determined by the single-ns-electron fractions of the moving ion and the strength of the fields B_{ns}, the product of which will increase with velocity as still deeper ion shells become involved in the electron-capture and -loss processes. Ultimately, as observed for C ions,[7] the transient field will decrease as the velocity becomes high enough that the innermost orbital is depleted. Sudden changes in the transient-field strength, as seen[6] around $Z=9$, can be attributed to resonances in the capture-loss cross sections. The observation that a time of the order of 10 fs is needed to equilibrate the $1s$ fractions might influence transient fields measured for very short-lived nuclei.[7]

The present study contradicts the interpretation of Zalm *et al.*[6] In the first place, it is very unlikely that the MO picture will be appropriate to describe capture at these high velocities of loosely bound Fe M and N electrons. Hence their arguments that the capture process is very selective in capture from the Fe $3d$ shell, giving rise to $\xi^{2s}\sim 0.3$, are rather dubious. Also, they claim that loss of Si $1s$ electrons will not occur, and the transient field is attributed entirely to polarized $2s$ electrons. The present measurements show that $1s$ vacancies *do* exist even at velocities as low as $4v_0$, and it is argued that they contribute significantly to the transient field.

Naturally, more experimental and theoretical investigations are needed in order to establish the detailed relation between transient fields and the electron configurations of the moving ions. However, as the understanding grows, transient-field measurements might turn out to provide valuable new information on the ion-solid interaction.

Thanks are due J. Chevallier for skillful target preparation. One of us (J.L.E.) wishes to thank the Hahn-Meitner Institute in Berlin for financial support.

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Observation of Sixfold Valley Degeneracy in Electron Inversion Layers on Si(111)

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(Received 30 November 1978)

We have observed the expected sixfold valley degeneracy in the inversion layer on Si(111). This observation suggests that the twofold valley degeneracy, observed in previous experiments, cannot be an intrinsic effect due to the intervalley charge-density–wave state proposed by Kelly and Falicov.

The first quantum mechanical treatment of the electron inversion layer on (111) surfaces of Si was given by Stern and Howard,[1] using the effective-mass approximation. They predicted a sixfold valley degeneracy for the ground-state subband. (Its two-dimensional constant-energy ellipses and the first Brillouin zone are illustrated in the inset of Fig. 1.) Experimentally, however, only twofold valley degeneracy was observed in previous studies of the Shubnikov–de Haas (SdH) effect.[2-5] Kelly and Falicov[6] first proposed that this lifting of the sixfold valley degeneracy manifested a charge-density-wave (CDW) state. In this so-called CDW-β state, four of the six electron valleys were coupled, through intervalley phonon exchange interactions, into two pairs. Each pair produced one occupied bonding state, and the resulting ground-state subband was twofold degenerate. Subsequently, Nakayama[7] proposed a triple-CDW state, in which three symmetrically located electron valleys were coupled with the other three to give rise to an occupied sub-band with a twofold valley degeneracy. The formation of such intervalley CDW states has also been invoked to explain a number of anomalies observed in the inversion layers on (100) as well as (111) surfaces when uniaxial stresses were applied to the Si substrates.[8-10]

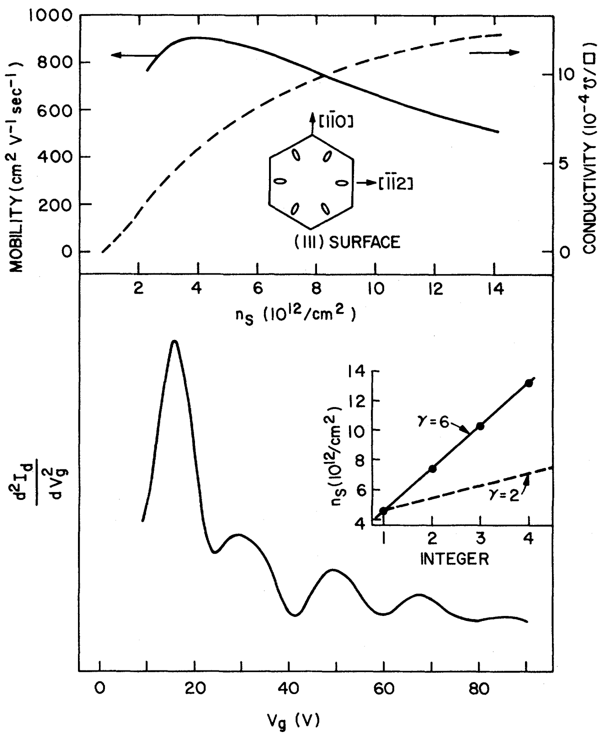

FIG. 1. Upper panel, the conductivity and mobility of an n-channel MOSFET's on (111) n-type Si at 4.2 K; lower panel, the Shubnikov–de Haas effect observed in d^2I_d/dV_g^2 as a function of V_g from the same device at 4.2 K with $B = 100$ kG applied perpendicular to the surface. The insets are explained in the text.