The influence of hydrogen diffusion on electrical resistivity of amorphous metallic alloys

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ABSTRACT

We discuss the determination of the diffusion coefficient of hydrogen in amorphous metallic structures with the use of changes of the electrical resistivity caused by hydrogen. The main contribution to resistivity in amorphous metallic structures due to hydrogen is made by the local shift of the structure factor $S(2k_F)$ in spatial areas saturated by hydrogen. We modeled numerically diffusion of the hydrogen from the infinitely thin hydrogenated layer in the middle of the infinite quasi-one-dimensional amorphous rod. The coefficient of diffusion of protons D=5.0·10^{-9} m^2/s in this model was set, and the aim was to obtain this coefficient from dependences of the dispersion of the distribution of resistivity on time. It is found that the coefficient of diffusion can be determined from data of electrical resistivity of amorphous metals except the case when $2k_F$ is in the vicinity of the position of the first maximum of the structure factor.

The model

The diffusion equation for diffusion from the infinitely thin layer was solved:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2};\quad \begin{matrix} c\to 0 \text{ at } |x|>0,\ t\to 0;\\ c\to\infty \text{ at } |x|\to 0,\ t\to 0\end{matrix}\qquad c(x,t)=\frac{\chi}{\sqrt{2\pi D t}}e^{-\frac{x^2}{4Dt}};\quad D=\frac{a^2}{\tau_0\cdot q}e^{-U/k_BT}.$$

The electrical resistivity of amorphous metal:

$$\rho(T)=\frac{30\pi^3\hbar^3}{\mu e^2 k_F^2\varepsilon_F\Omega_c}\sin^2[\eta_l(\varepsilon_F)]\cdot S(2k_F),$$

$S(2k_F)=1+[a(2k_F)-1]e^{-2[W_{k_F}(T)-W_{k_F}(0)]}$, $W(T)$ is the Debye-Waller factor,

$$a(k\sigma)=\left[1-c'^{(k\sigma)}\right]^{-1},\quad c'(k\sigma)=-4\pi\sigma^3\int_0^1 ds\cdot s^2\frac{\sin(sk\sigma)}{sk\sigma}f(s),$$

$a(k\sigma), c'(k\sigma)$ and $f(s)$ were calculated according to the solution of the Percus-Yevick equation for the hard-sphere model with the packing-density parameter 0.525.

$\frac{\Delta\rho}{\rho_0}\sim\frac{\Delta S}{S_0}$, where S_0 is the structure factor of the amorphous metal without hydrogen, ρ_0 is resistivity of the metal without hydrogen.

The molar volume and $2k_F$ change with changes of $c(x)$:

$$V_{mol}(x,c)=V_{mol}(x,c=0)\left(1+\alpha\cdot c(x)\right);$$

$$k_F=\left[2\pi^2 N_A\cdot Z/V_{mol}\right]^{1/3};\quad k_F(c)=k_F(c=0)\left[\frac{1}{1+\alpha\cdot c}\right]^{1/3}$$

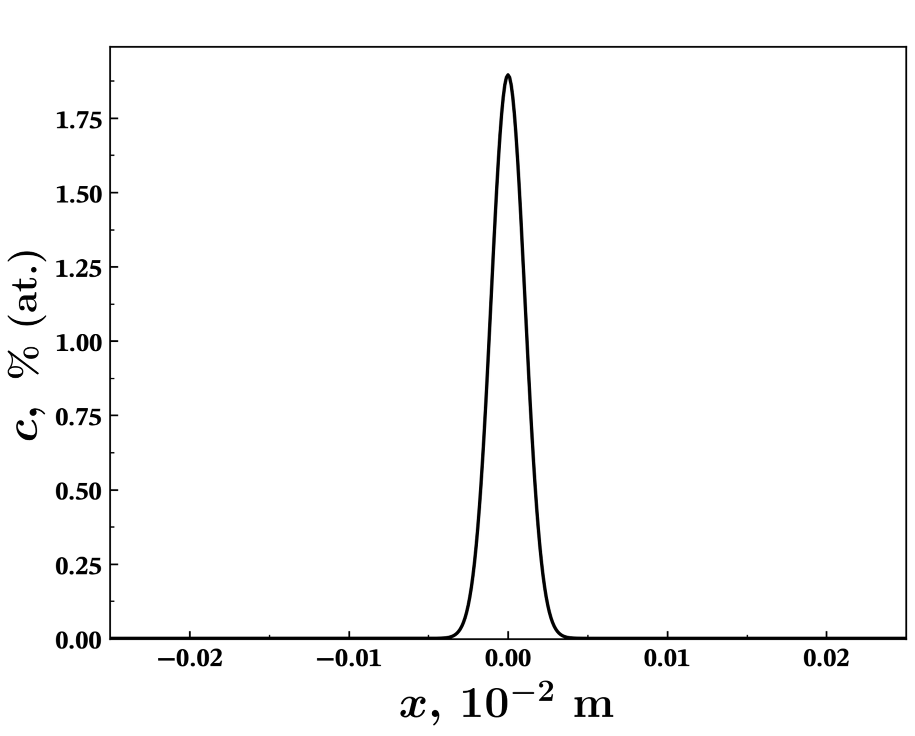
$$\overline{X^2}(t)=\frac{\int_{L/2}^{L/2}x^2c(x,t)dx}{\int_{-L/2}^{L}c(x,t)dx};\quad \overline{X^2}(t)=2Dt;\quad \overline{X^2}(t)=\frac{\int_{-L/2}^{L/2}x^2\frac{\Delta S}{S_0}(x,t)dx}{\int_{-L/2}^{L/2}\frac{\Delta S}{S_0}(x,t)dx}$$

The aim of the work is to calculate D from dependences $\overline{X^2}(t)$ obtained with the use of distributions $\frac{\Delta S}{S_0}(x,t)$.

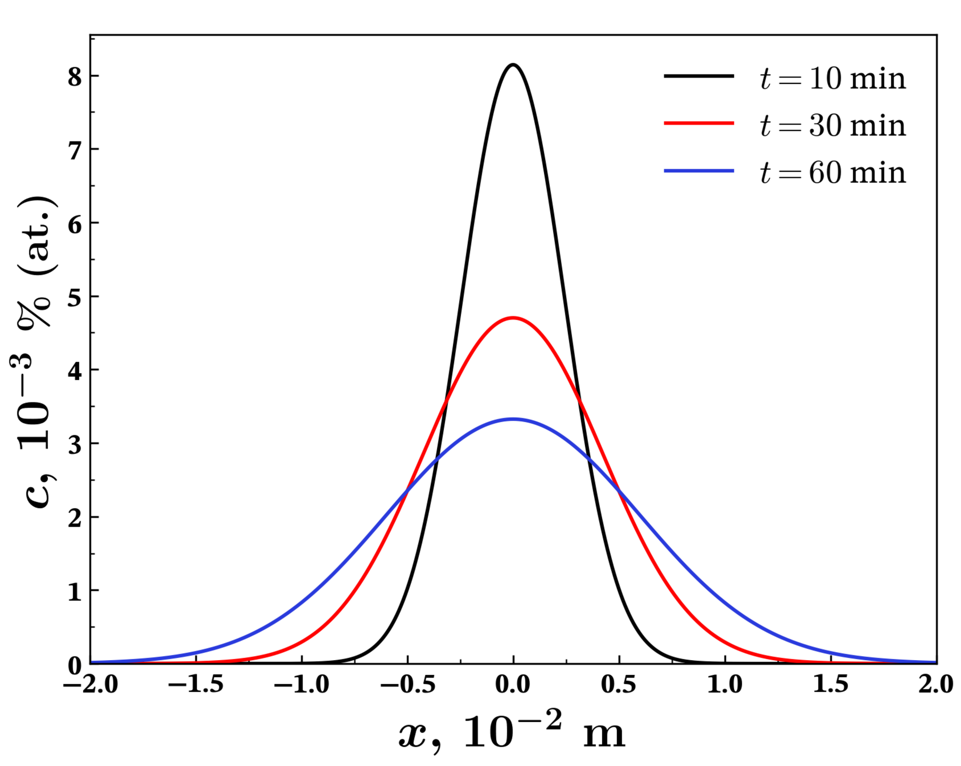
Parameters of calculations:

$T=300$ K, $D=D_0e^{-\frac{U}{k_BT}}$, $D_0=3.1\cdot10^{-8}$ m^2/s, $U=0.045$ eV, $D=5.00\cdot10^{-9}$ m^2/s, $\alpha=0.16$, $\sigma=2.5\cdot10^{-10}$ m, $c_0=1.9$ % (at.).

Distributions of hydrogen along the sample:

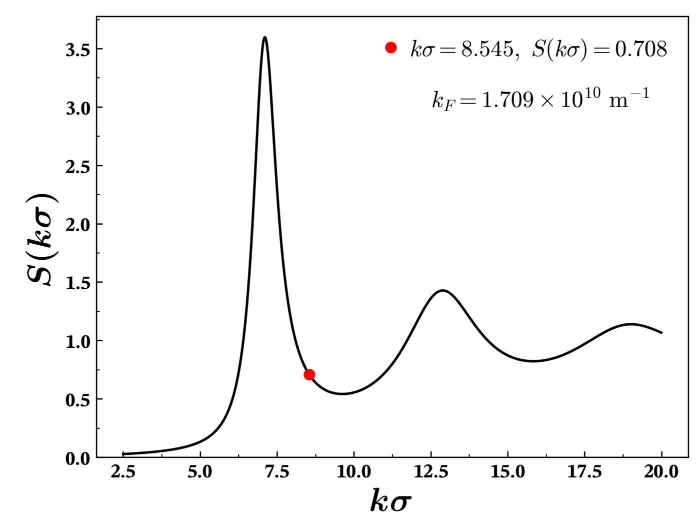


The initial distribution of concentrations

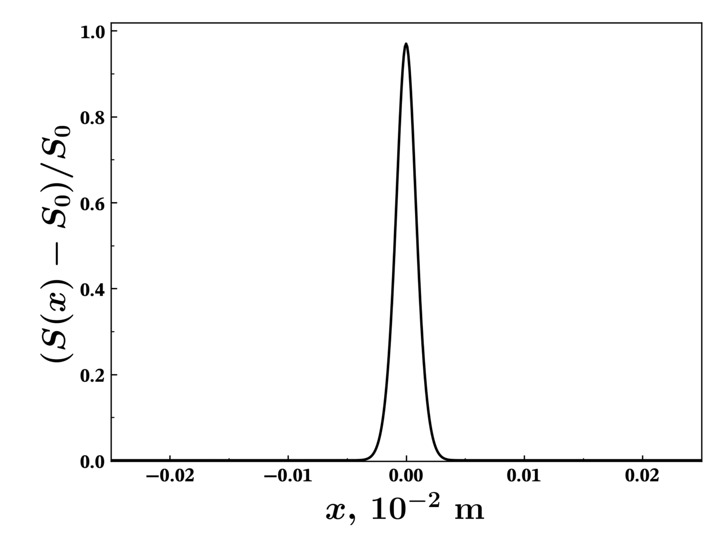


Distributions of concentrations during diffusion

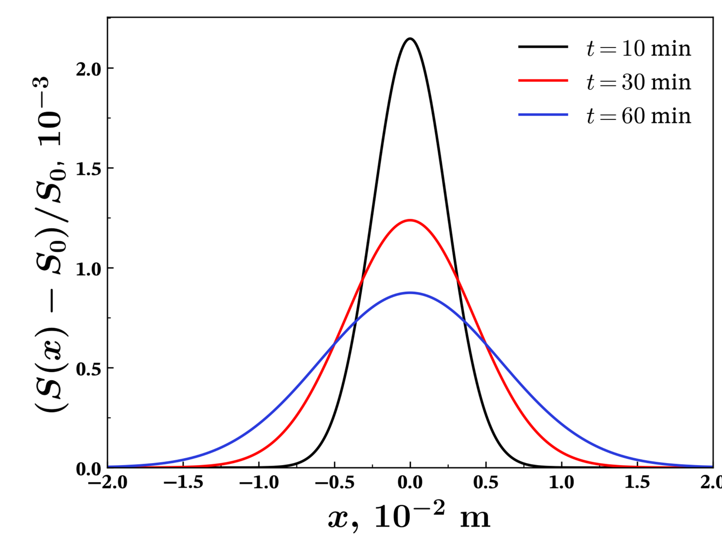
Results of calculations for $2k_F(c=0)>k_p$:



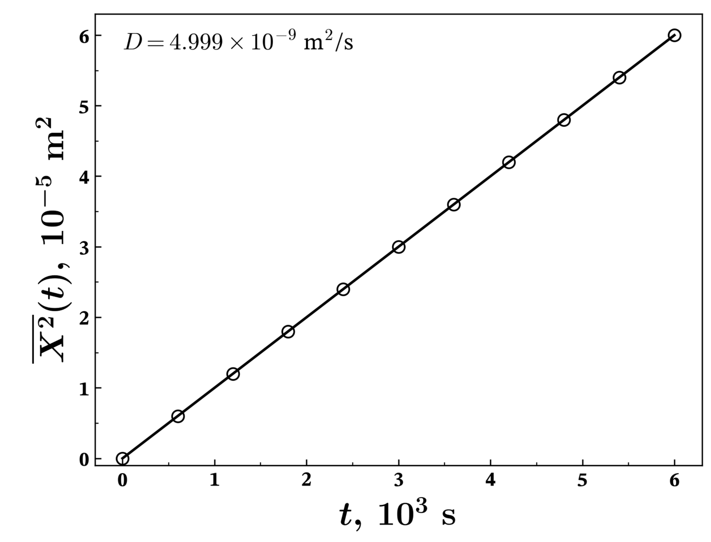
The value of $2k_F$ is shown by the red dot



The initial distribution $(S(x)-S_0)/S_0$

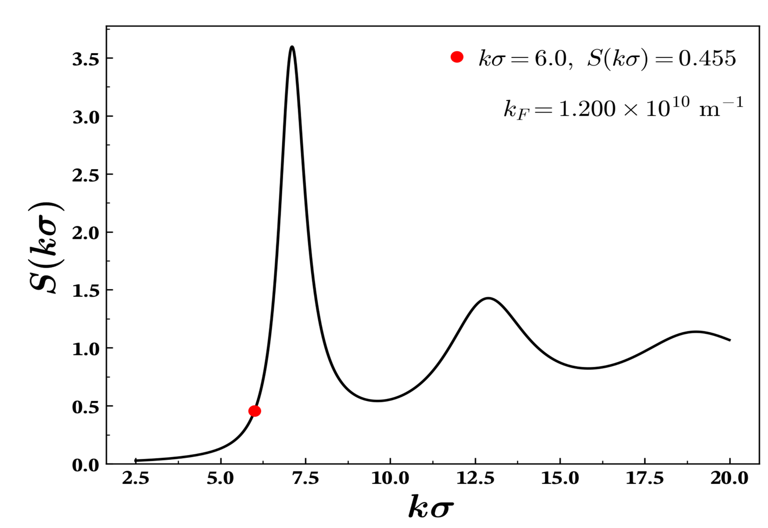


Distributions $(S(x)-S_0)/S_0$

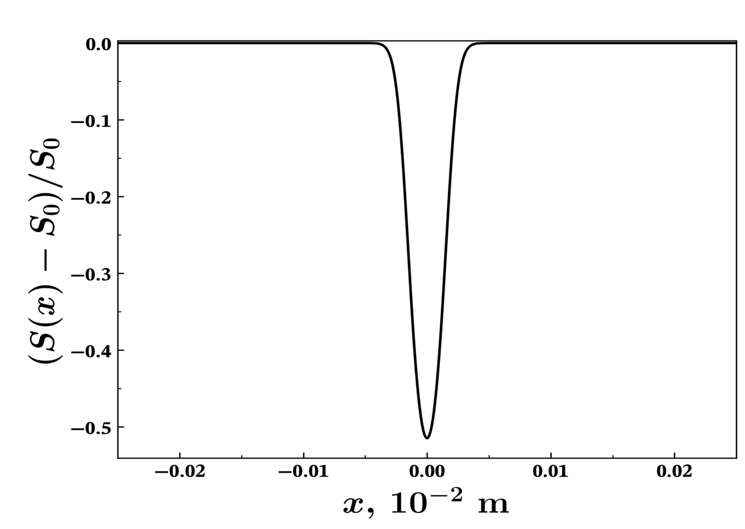


The slope of $\overline{X^2}(t)$ is equal to $4.999\cdot10^{-9}$ m^2/s

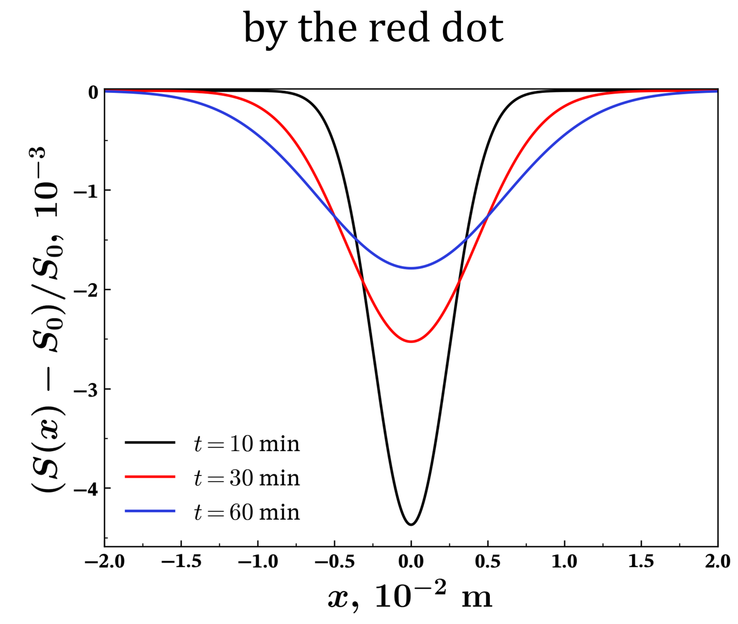
Results of calculations for $2k_F(c=0)<k_p$:



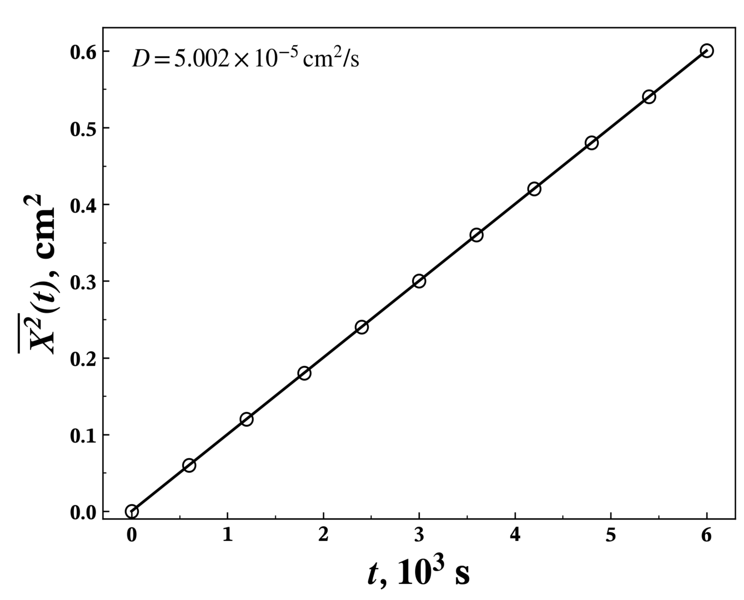
The value of $2k_F$ is shown by the red dot



The initial distribution $(S(x)-S_0)/S_0$< 0

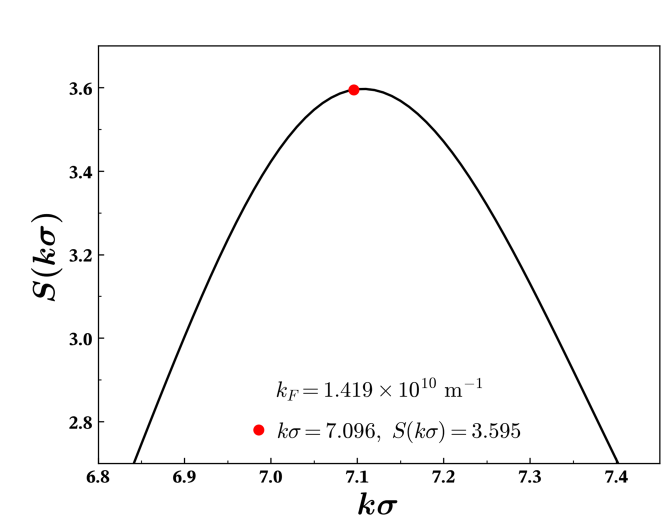


Distributions $\frac{(S(x)-S_0)}{S_0}<0$ during diffusion

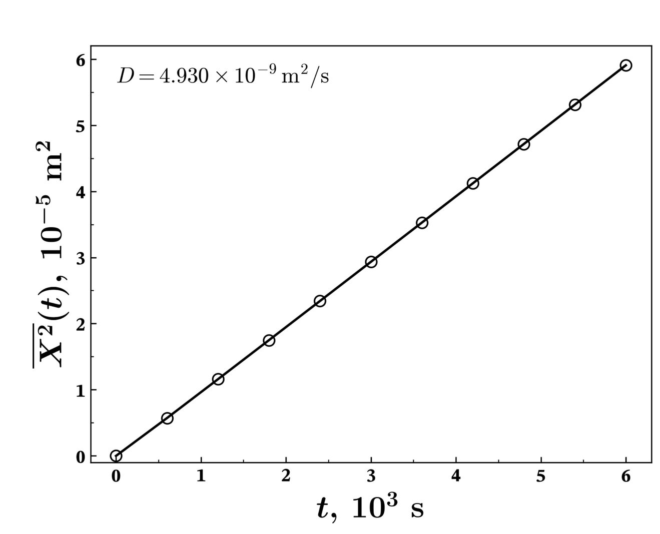


The slope of $\overline{X^2}(t)$ is equal to $5{,}002\cdot10^{-9}$ m^2/s

Results of calculations for $2k_F(c=0)\sim k_p$:



The value of $2k_F$ is shown by the red dot



The slope of $\overline{X^2}(t)$ is equal to $4.930\cdot10^{-9}$ m^2/s

CONCLUSIONS

1. **We found that in ranges of the supposition that $\frac{\Delta S(2k_F)}{S(2k_F)}\sim\frac{\Delta\rho}{\rho}$, at $2k_F > k_p$ the presence of hydrogen caused an increase of resistivity, so $\Delta\rho/\rho_0 > 0$, whereas at $2k_F < k_p$ we obtained $\Delta\rho/\rho_0 < 0$. In both these cases we obtained the correct coefficient of diffusion D of hydrogen from dependences of the dispersion of distributions of $\frac{\Delta S(2k_F)}{S(2k_F)}$ on time ($\overline{X^2}=f(t)$).**
2. **We discussed the special case $2k_F \sim k_p$, when the deviation of the calculated value of the diffusion coefficient from the set value D becomes large.**
3. **Thus, we demonstrated that the coefficient of diffusion of hydrogen in the amorphous metal can be calculated from spatial distributions of changes of the resistivity caused by hydrogen except the case when $2k_F \sim k_p$.**