RADIATION EFFECTS IN NANOSIZED CLUSTERS

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ABSTRACT

In this communication we present results of computer simulation of radiation-enhanced processes in nanosized ferromagnetic clusters under the irradiation by elementary particles and ions. Dynamic defects and possibility of their experimental monitoring are considered. Radiation resistance of nanostructured materials is characterized by the size of instability region for knocked-out atom. Heating and thermoelastic effects on defect structure and materials functionality are discussed.

Key words: magnetic nanocluster, irradiation, defects.

INTRODUCTION

Application of magnetic nanomaterials for data storage and recording devices makes it possible to increase writing density in 104 times. Data record is made in separate nanosized single-domain particle with two energy states corresponding to magnetic moment orientation and separated by potential barrier. Significant advantages and perspective applications of these data carriers determine intensive development of this scientific and technological direction [1-4].

Magnetic nanoclusters are formed by different physical- and chemical-based techniques. For example, injection of metallic powder (Fe, Ni, Co) to dense compression plasma with temperature 2-3 eV [5-6] results in the formation of metallic vapor that condenses under certain thermodynamic conditions (*Fig. 1*). Deposition of metallic vapor on the substrate lets to the formation of metal layer consisting of spherical clusters with multi-level structure: submicron clusters (0,1-0,2 μm radius) are formed from a number of nanosized ones (10-25 nm radius).

Magnetic nanostructured cluster arrays have great prospects in the development of new generation of devices for operation in open space conditions. Nevertheless, the problem of their radiation stability is still insufficiently studied.

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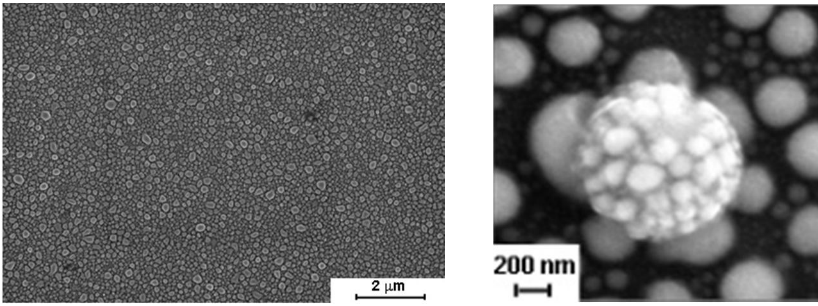

(a) (b)

Fig. 1 – Scanning electron microscopy images (20k and 150k magnification) of iron clusters deposited from dense compression plasma on silicon surface

DYNAMIC RADIATION EFFECTS

Let us consider atom dynamics in the substance irradiated by changed and neutral particles (protons, ions, electrons, neutrons). Assume that atom with mass M is knocked-on by incident particle (or other displaced atom) and has kinetic energy W (W is less than defect formation energy Ed). It's motion is described by the following expression:

$$\frac{d^2\rho}{dt^2}+\xi\frac{d\rho}{dt}+f(\rho)=0 \quad (1)$$

where ρ – distance from atom to lattice point; $\xi = n\cdot\Im$; n – number of force interactions between moving atom and lattice atoms; $\Im$ – number of electrons in a cylinder with base Σ and height $\upsilon_a = d\rho/dt$ ($\Sigma \sim \pi r_0^2$, r_0 – covalent atomic radius);

$$f(\rho)=-\frac{1}{M}\frac{dU(\rho)}{d\rho} \quad (2)$$

$$U(\rho)=\sum_{i,j}\frac{e^2 i\cdot j}{\varepsilon_0\varepsilon\rho}\varphi_{ij} \quad (3)$$

φ_{ij} – probability of "vacancy-interstitial atom" system to have configuration with charge states i and j, respectively, ε_0 – electric constant, ε – material permittivity, e – elementary charge.

Fig. 2 shows results of computer simulation of the process described by eq. (1) for iron atom with initial kinetic energy W=50 eV.

Dynamic state of vacancy and interstitial atom results in generation of electromagnetic radiation pulse. Its power I is proportional to the acceleration of interstitial atom w

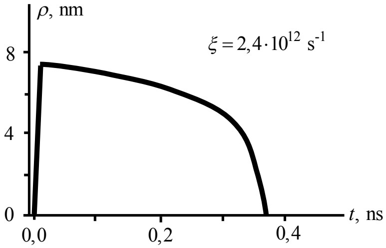

Fig. 2 – Time dependence of the distance between iron atom and lattice point

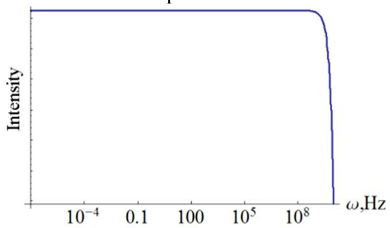

Fig. 3 – Electromagnetic radiation spectrum of dynamic defect generated by knocked-out iron atom with initial energy 50 eV

$$I \sim w^2(t) \tag{4}$$

Fourier transformation of (4) subject to atom's motion law (1) gives electromagnetic radiation spectrum shown on *Fig. 3*. Thus, dynamic defects under the irradiation of materials by elemental particles and ions can be registered by the analysis of electromagnetic spectral composition.

Life time of the dynamic defect is about 10^{-10}c that is three orders greater than Debye period of lattice atoms oscillations. Therefore, acoustic lattice relaxation in this region results in the formation of shock pressure P propagating radially in cluster volume. Consider displacement cascade to be a sphere with radius R. At the moment $t = 0$ rectangular "velocity pulse" υ_0 is generated by m dynamic defects

$$\upsilon_0 = \left(\frac{2MW}{\gamma \cdot B}\right)^{1/2} \frac{m\xi}{4\pi R^2} \tag{5}$$

where γ – material density, B – bulk modulus. Velocity of deformation propagation υ is obtained from nonlinear equation for mass velocity.

In the interaction of medium disturbance and dynamic defect (with deformation volume ω_0) the latter is affected by force $\vec{F} = -\gamma u \omega_0 \vec{\nabla} \upsilon$ (where u – speed of velocity in the matter). On the other hand, $\vec{F} = \vec{P} \cdot \delta$, where $\vec{P} = \gamma \cdot u\vec{\upsilon}$, δ – scattering cross-section

$$\delta = \left[\frac{2(1+\nu)\omega_0 G}{3(1-\nu)\pi^2 B} \ln\frac{R_d}{r_d}\right]^2 \sum_i K_i^4 \tag{6}$$

where ν – Poisson's ratio, G – shear modulus, R_d – radius of the region deformed by the defect, r_d – defect radius, K_i – wave vector magnitude of the i-th spectral component of the deformation pulse, ω_0 – dilation volume. For body-centered iron lattice $F \sim 10^{-11} \div 10^{-10}$ N. Energy Q, obtained by the defect is estimated by the expression

$$Q = \frac{(F \cdot \tau)^2}{2M_d} \tag{7}$$

where τ – time of interaction between deformation pulse and defect with mass M_d $\left(\tau \sim 10^{-12}\ \text{s}\right)$.

When F > F_0 and $Q > E_m$ (where F_0 is critical force equal to U_a/a; U_a – activation energy; *a* – lattice parameter; E_m – migration energy) one obtains diffusionless motion of the defect to nanoparticle surface (for iron $F_0 \sim 7 \cdot 10^{-12}\ \text{N}$). One should take into account that thermal heating of the cluster results in activation of diffusion processes. Diffusion length $\sqrt{D\tau_p}$ (*D* – diffusion coefficient, τ_p – heating time) may exceed cluster size. For $D \sim 4 \cdot 10^{-4}\ \text{m}^2/\text{s}$ $(T \sim 1200 \div 1500\ \text{K})$ and "temperature life time" $\tau_p \sim 10^{-12}\ \text{s}$ one obtains $\sqrt{D\tau_p} \sim 2 \cdot 10^{-8}\ \text{m}$, $Q \sim 1{,}5 \div 6{,}0\ \text{eV}$.

Since kinetic energy of incident particle transforms to atoms displacement and heating of the deceleration region, we consider displacement cascade to be an instant heat source with temperature field *T*(*r*, *t*) (*Fig. 4*). Radial thermoelastic stresses $\sigma_{rr}(r, t)$ and their gradient were calculated as

$$\sigma_{rr}(r,t) = 4\mu\alpha \frac{3\lambda + 2\mu}{\lambda + 2\mu} \left\{ \frac{1}{R_k^3} \int_0^{R_k} T(r,t) \cdot r^2 dr - \frac{1}{r^3} \int_0^{r} T(r,t) \cdot r^2 dr \right\}, \tag{8}$$

where μ and λ are Lamé coefficients, α – linear expansion coefficient, R_k – cluster radius.

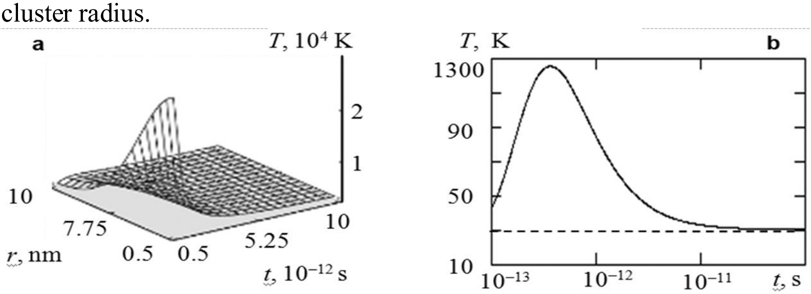

Fig. 4 – Space-time temperature distribution (a) and temperature evolution at *r* = 7 nm (b) for point heat source in iron nanocluster (R_k = 15 nm)

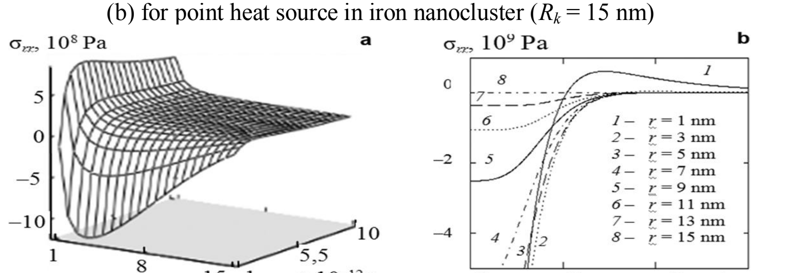

Fig. 5 – Space-time distribution of radial thermoelastic stresses (a) and stress evolution (b) in spherical iron nanoparticle (R_k=15 nm)

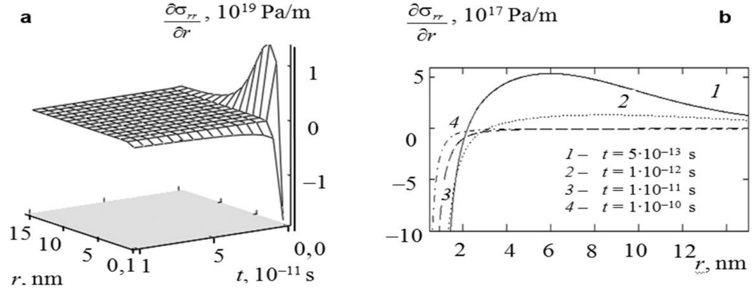

Fig. 6 – Space-time distribution of radial thermoelastic stresses gradient (a) and their evolution (b) in spherical iron nanoparticle (R_k=15 nm)

Fig. 5-6 show that elastic, thermal and thermoelastic response of cluster on radiation-induced structural changes results in defects elimination in nanoparticle (in this case Le Chatelier-Broun principle works in a special way).

Radiation-induced heating affects magnetic properties of nanocluster. Let us consider barrier height V between stable and metastable magnetic states of the ferromagnetic nanocluster (the value of V, obviously, determines stability of the recorded information). According to [7] it is estimated from the following expression:

$$V = \frac{4\pi R_k^3 K_{\text{eff}}}{3}\left[1 - \frac{H}{H_c}\right]^2 \tag{9}$$

where H – external magnetizing force; H_c – coercive force; K_{eff} – effective magnetic anisotropy constant. Temperature dependence of K_{eff}, is expressed in the following manner [2]:

$$K_{\text{eff}} = \frac{4\pi\mu_0 (H_c)_{\max} J_s(0)}{2}\left(1 - B_J T^b\right) \tag{10}$$

where $(H_c)_{\max}$ – theoretical limit of coercive force; $J_s(0)$ – saturation magnetization for $T = 0$; B_J and b are values determined by cluster material and size.

In the absence of external magnetic field $V = V_0$:

$$V_0(T) = \frac{8\pi^2 \mu_0 R_k^3 (H_c)_{\max} \cdot J_s(0)}{3}\left[1 - B_J T^b\right] \tag{11}$$

Calculations performed for experimental data [2] on iron clusters with $R_k \geq 7$ nm with extrapolation to high temperature regions give following values: $B_J = 4{,}76 \cdot 10^{-5}\ \text{K}^{-3/2}$; $b = 1{,}5$; $J_s(0) = 6{,}58 \cdot 10^4$ A/m; $(H_c)_{\max} = 4{,}78 \cdot 10^4$ A/m. *Fig. 7* shows temperature dependence of potential barrier height V_0.

Thus, V0 turns to zero at temperature T ≈ 760 K that is less than Curie temperature of bulk iron (TC = 1044 K [8]).

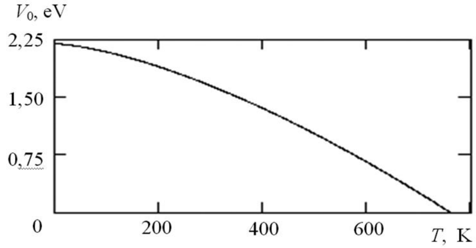

Fig. 7 – Temperature dependence of potential barrier height V_0 between magnetic states of iron nanocluster (R_k=7 nm)

Calculation results show that temperature of the nanocluser under irradiation is higher than temperature of magnetic transition (when V0=0). Therefore, it results in failure of information record in the nanosized memory elements. This effect becomes more considerable for small-sized clusters.

CONCLUSIONS

1. Dynamic radiation defects that affect defect-impurity system of the cluster can be examined by electromagnetic radiation spectrum.
2. Irradiation of nanoszied particles under the irradiation by charged and neutral particles results in radiation-enhanced self-organization tending to minimize bulk imperfection.
3. Temperature rise in nanoparticles under irradiation is one of the most significant factors that determine radiation stability of nanosized memory elements.

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