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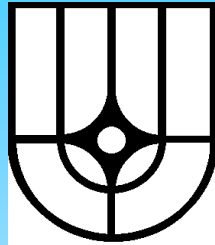
**Joint ICTP-IAEA Advanced Workshop on Multi-Scale Modelling for
Characterization and Basic Understanding of Radiation Damage
Mechanisms in Materials**

12 - 23 April 2010

Radiation growth of amorphous alloys under heavy ion irradiation

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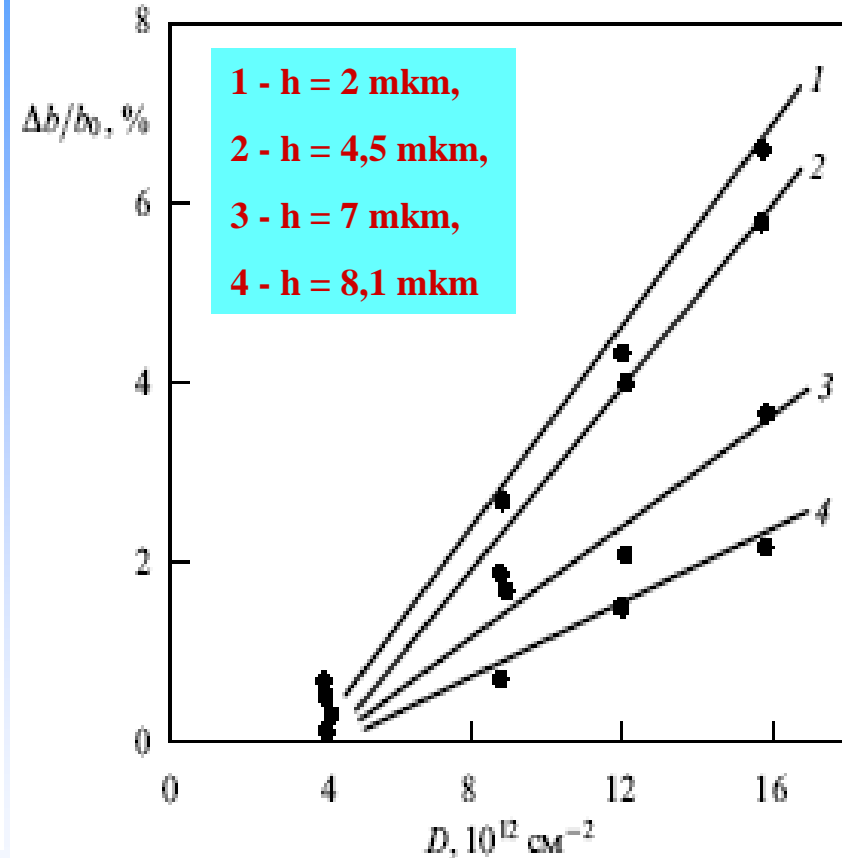
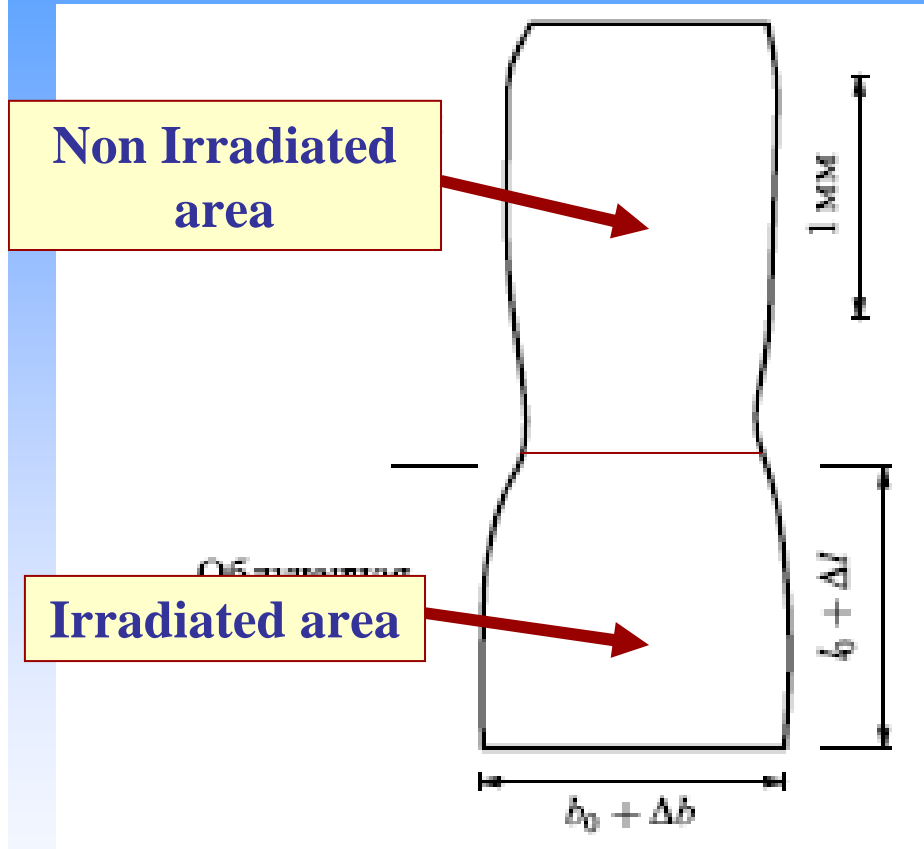


**Theoretical Modeling of Radiation Growth of
Amorphous Alloys under Heavy Ion Irradiation**

A.I. Ryazanov

**Joint ICTP/IAEA Advanced Workshop on Multi-Scale Modelling for Characterization and
Basic Understanding of Radiation Damage Mechanisms in Materials
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Radiation Growth in Amorphous Alloys under Heavy Ion Irradiation



Amorphous alloy irradiated by Xe ions with the energy $E = 1,34 \text{ MeV/n}$

Main peculiarities of radiation growth in amorphous alloys under heavy ion irradiation

(1) Large anisotropic variations of the sample dimensions are produced by irradiation. The anisotropy is induced by the incident particle beam (the growth direction is normal to the beam direction).

(2) These dimensional changes start from incubation dose B , reach 10%, and do not saturate with irradiation dose.

(3) The effect strongly depends on the irradiation temperature.

(4) The effect is observed both in amorphous metallic alloys and in covalently bonded amorphous solids.

(5) A correlation between the magnitude of the effect and the electronic energy loss $\langle S_e \rangle$ has been observed.

Viscoelastic isotropic media for description of radiation growth of amorphous alloys

$$\sigma_{ik} = -K\alpha T\delta_{ik} + Ku_{ll}\delta_{ik} + 2\mu \left[u_{ik} - u_{ll} \frac{\delta_{ik}}{3} \right] + \xi \dot{u}_{ll}\delta_{ik} + 2\eta \left[\dot{u}_{ik} - \dot{u}_{ll} \frac{\delta_{ik}}{3} \right], \quad (1)$$

$$u_{ik} = \frac{1}{2} \left[\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} \right].$$

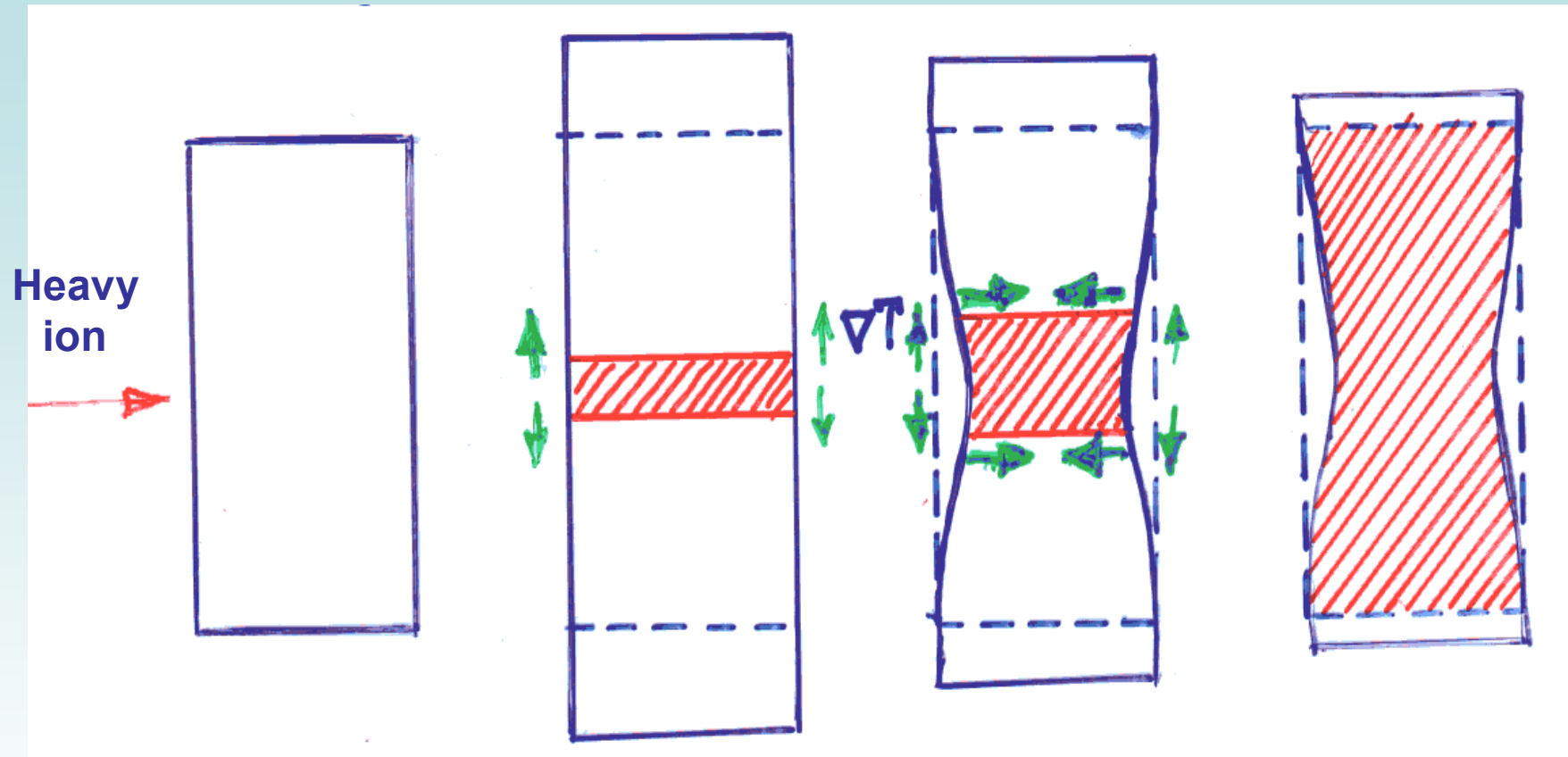
Here K is the bulk modulus, μ is the shear modulus, ξ is the bulk viscosity, η is the shear viscosity, $T = T_i - T_{irr}$, T_i is the ion temperature, α is the thermal expansion coefficient, u_{ik} is the strain tensor, \mathbf{u} is the displacement vector in the deformed material, and δ_{ik} is the Kronecker symbol. The Einstein summation rule is assumed in Eq. (1).

Substituting the stress tensor σ_{ik} (1) into the equation of motion for a small material volume, we have

$$\rho(d^2\mathbf{u}_i/dt^2) = \partial\sigma_{ik}/\partial x_k,$$

where ρ is the material density.

Mechanisms of anisotropic radiation growth of amorphous alloys under heavy ion irradiation



$$t = t_0 = 0,$$

$$T = T_0$$

$$t \leq \tau_{ep},$$

$$\sigma_T \propto \alpha \nabla T_i,$$

$$\frac{d\varepsilon}{dt} \approx \frac{1}{\eta_{irr}} \sigma_T$$

$$t \leq \tau_{ep} = \frac{4R_T^2}{\chi_e},$$

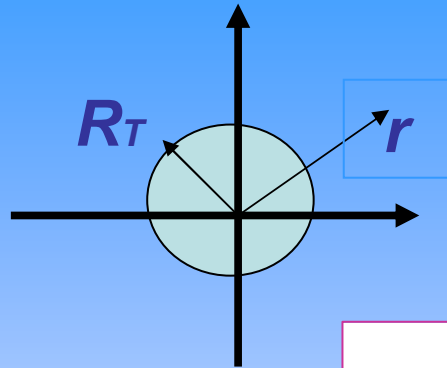
$$\rho = Const,$$

$$div \vec{u} = 0$$

$$t \geq t_c,$$

$$\eta = \eta_{irr}$$

1. "Hot" stage of material atoms near track area



$$t \leq \tau_C = 4R_T^2 / \chi_i$$

$$T(r, t) = \frac{T_0 R_T^2}{(R_T^2 + 4\chi_i t)} \times \exp[-r^2 / (R_T^2 + 4\chi_i t)]$$

We take initial conditions

$$u_r(r, 0) = u_0 r \exp(-r^2 / R_l^2)$$

$$\dot{u}_r(r, 0) = \dot{u}_0 r \exp(-r^2 / R_v^2)$$

Here R_l and R_v are characteristic dimensions of the regions where the initial ion displacements and initial ion momenta appear, respectively; u_0 and \dot{u}_0 are constants which can be obtained, e.g., from the Coulomb explosion and the electron blow models.

$$\eta = \eta_h$$

2. “Cold” stage of material atoms near track area

$$t \geq \tau_c = 4R_T^2 / \chi_i$$

$$u_r^c(r, 0) = u_r^h(r, t_c^i), \quad \dot{u}_r^c(r, 0) = 0$$

$$\eta = \eta_c$$

3. Irradiation Growth Rate of Amorphous Alloys

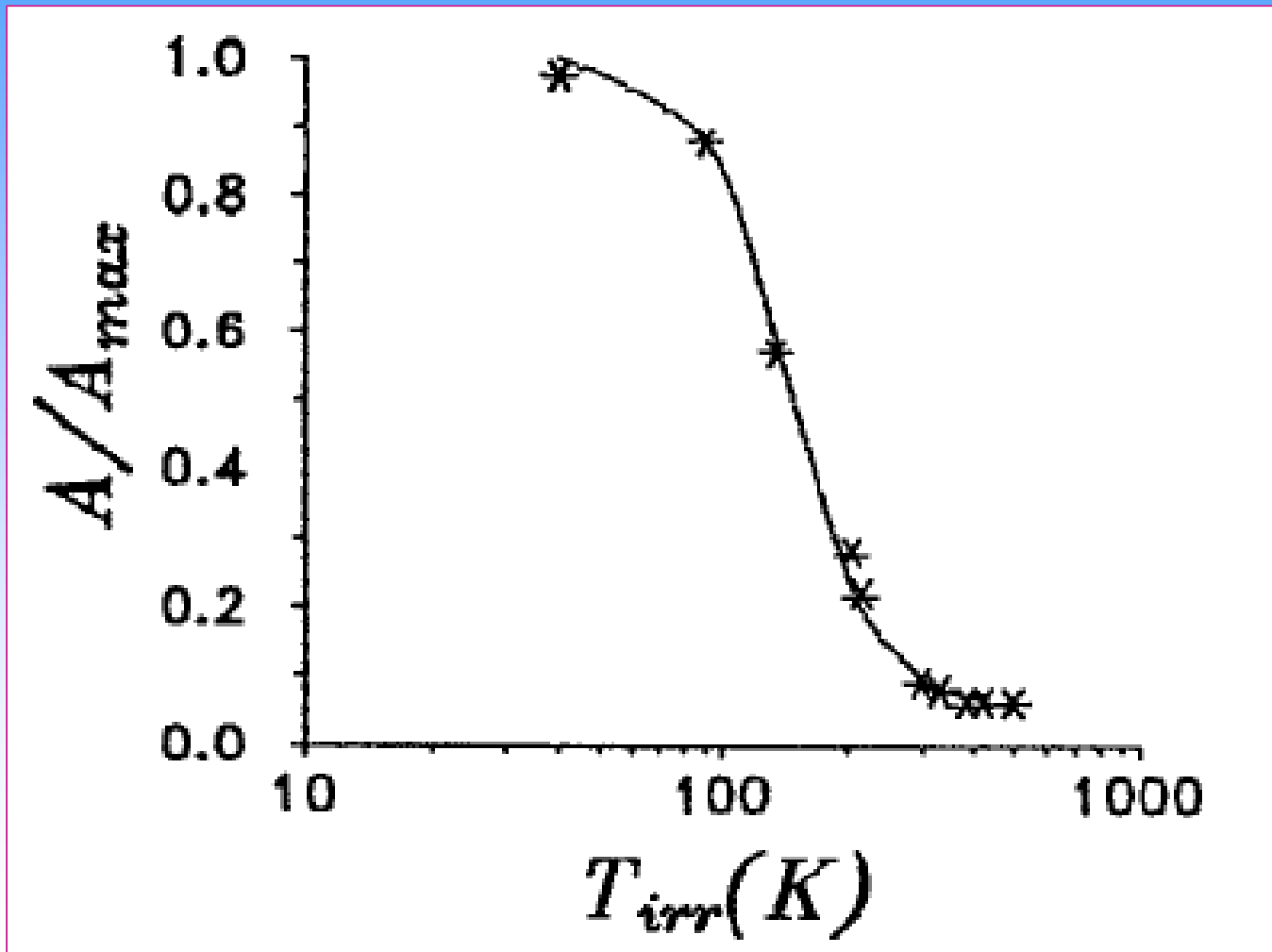
$$A = j^{-1} \frac{d}{dt} \left(\frac{\Delta b}{b} \right) = \frac{T_0 K \alpha R_T^4}{2 \chi_i \eta_h} \exp \left(-\frac{\mu \tau}{\eta_c} \right)$$

$$\frac{A}{A_{\max}} \approx \exp \left[-\frac{T^*}{T_{\text{irr}}} \exp(-G / T_{\text{irr}}) \right]$$

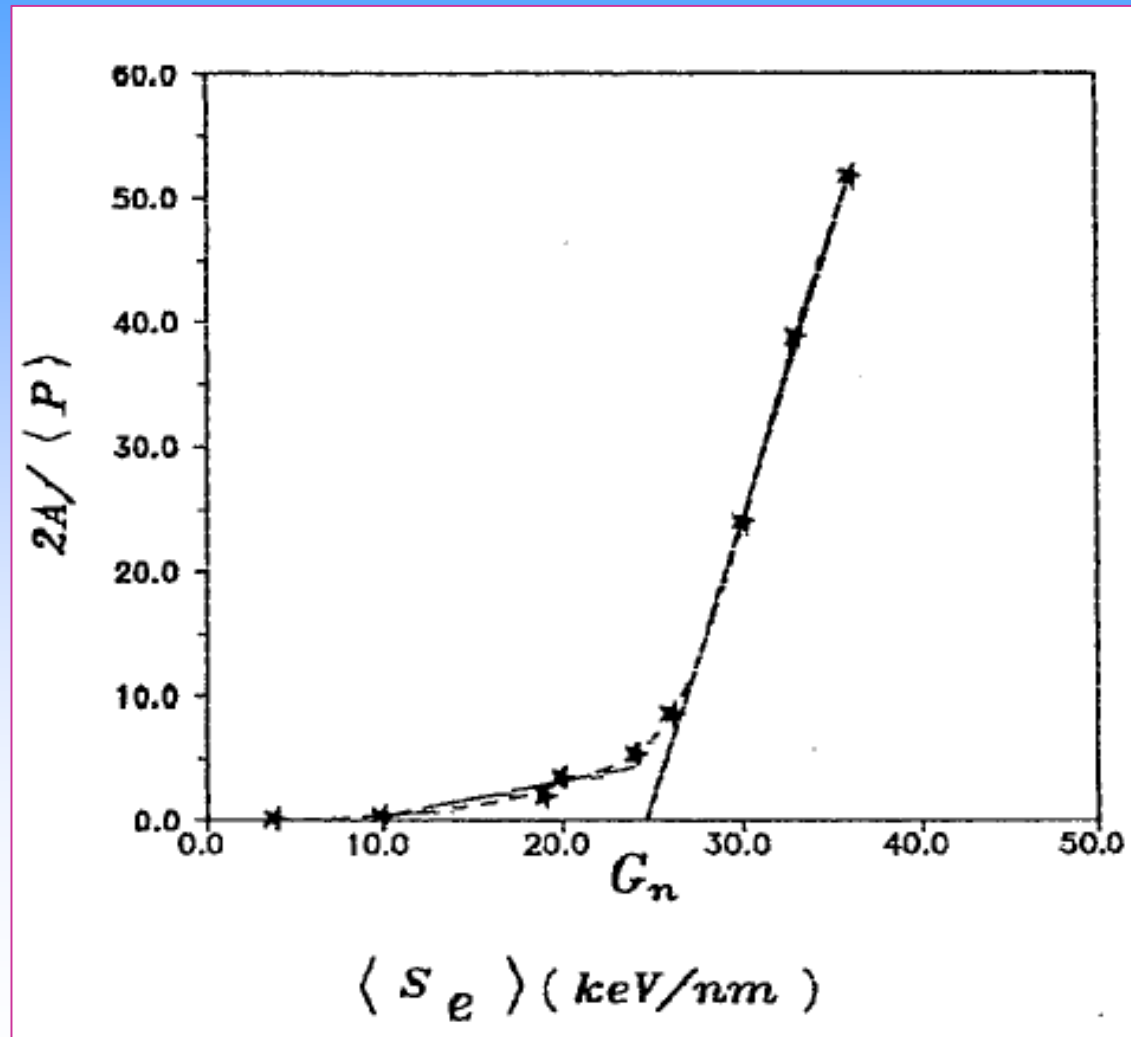
$$T^* = 4024K, G = 530K, (Pd_{80}Si_{20})$$

A.I.Ryazanov, A.E.Volkov, S.Klaumunzer, Phys.Rev.B,51 (1995) 12107

Experimental (*) and theoretical dependencies (-) of the deformation rate of versus irradiation temperature. ($A_{max} = 5.5 \times 10^{-15} \text{ cm}^2$ for $\text{Pd}_{80}\text{Si}_{20}$)

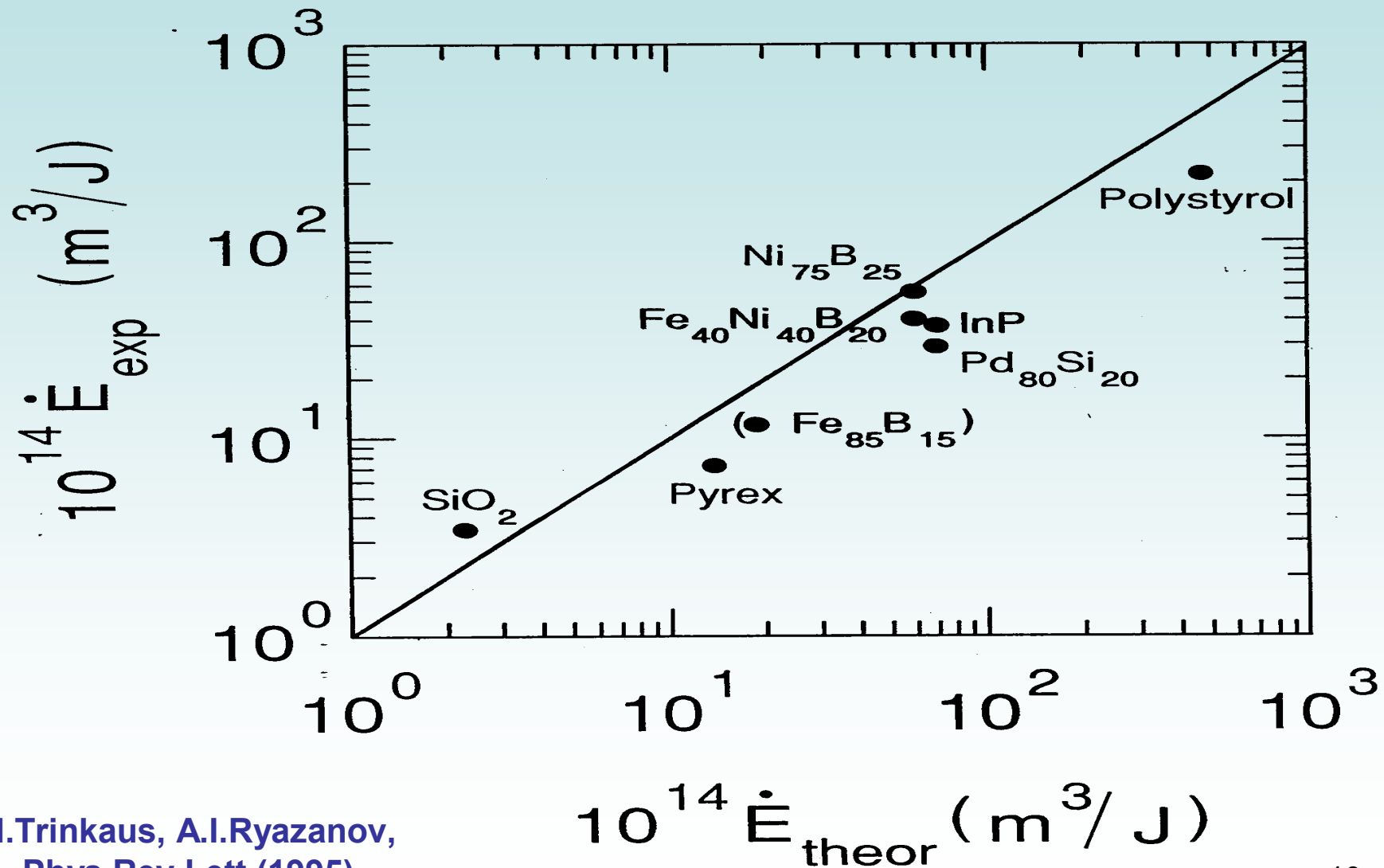


Experimental (*) and theoretical dependencies (-) of the irradiation growth rate of Pd80Si20 normalized to the total displacement cross-section $\langle P \rangle$ as a function of electron energy loss $\langle S_e \rangle$



Correlation between experimental and theoretical values of the normalized strain rate

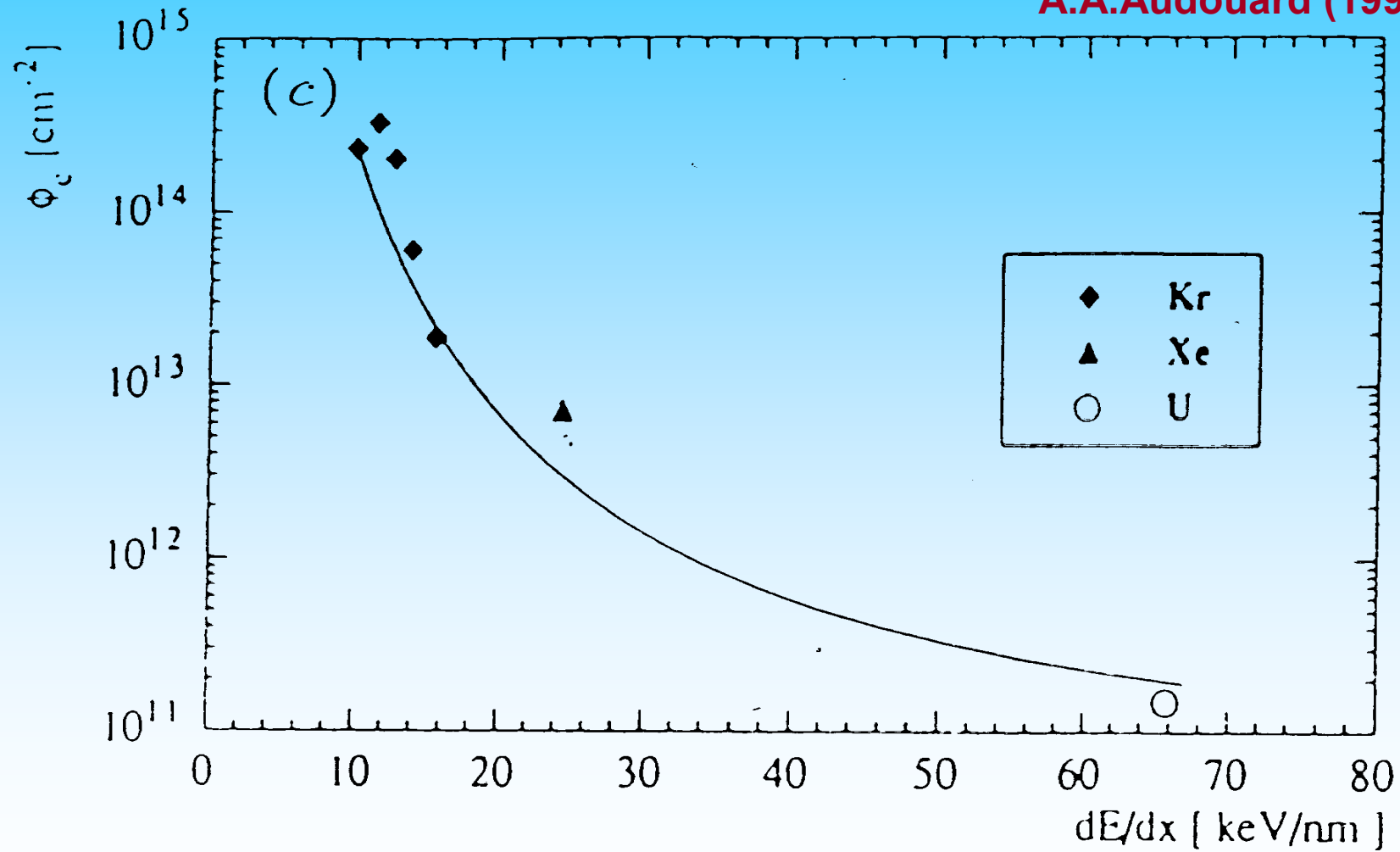
$$\dot{E} = \phi^{-1} d\dot{\epsilon}/dS_e$$



H.Trinkaus, A.I.Ryazanov,
Phys.Rev.Lett.(1995)

Experimental data for incubation dose for radiation growth of Fe₈₅B₁₅ as a function of electronic loss

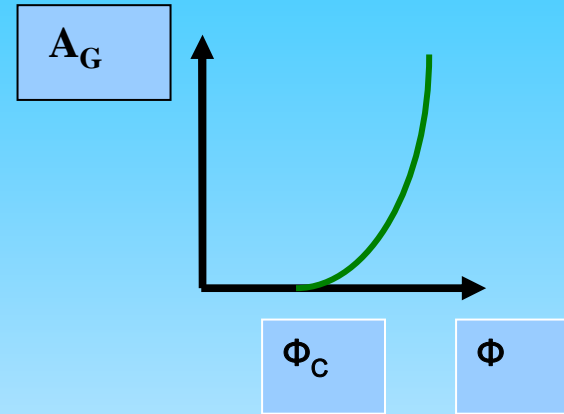
A.A.Audouard (1993)



Incubation dose for radiation growth of amorphous alloys

$$A_G \propto 1 / \eta_{irr}$$

$$T_{irr} = T_0 + \Delta T_0(S_e)$$



ΔT_0 - the maximum temperature increase in track area

$$\Delta T_0 = S_e / (3\pi n_a k_B R_T^2)$$

τ_σ - the characteristic time for shear stress relaxation

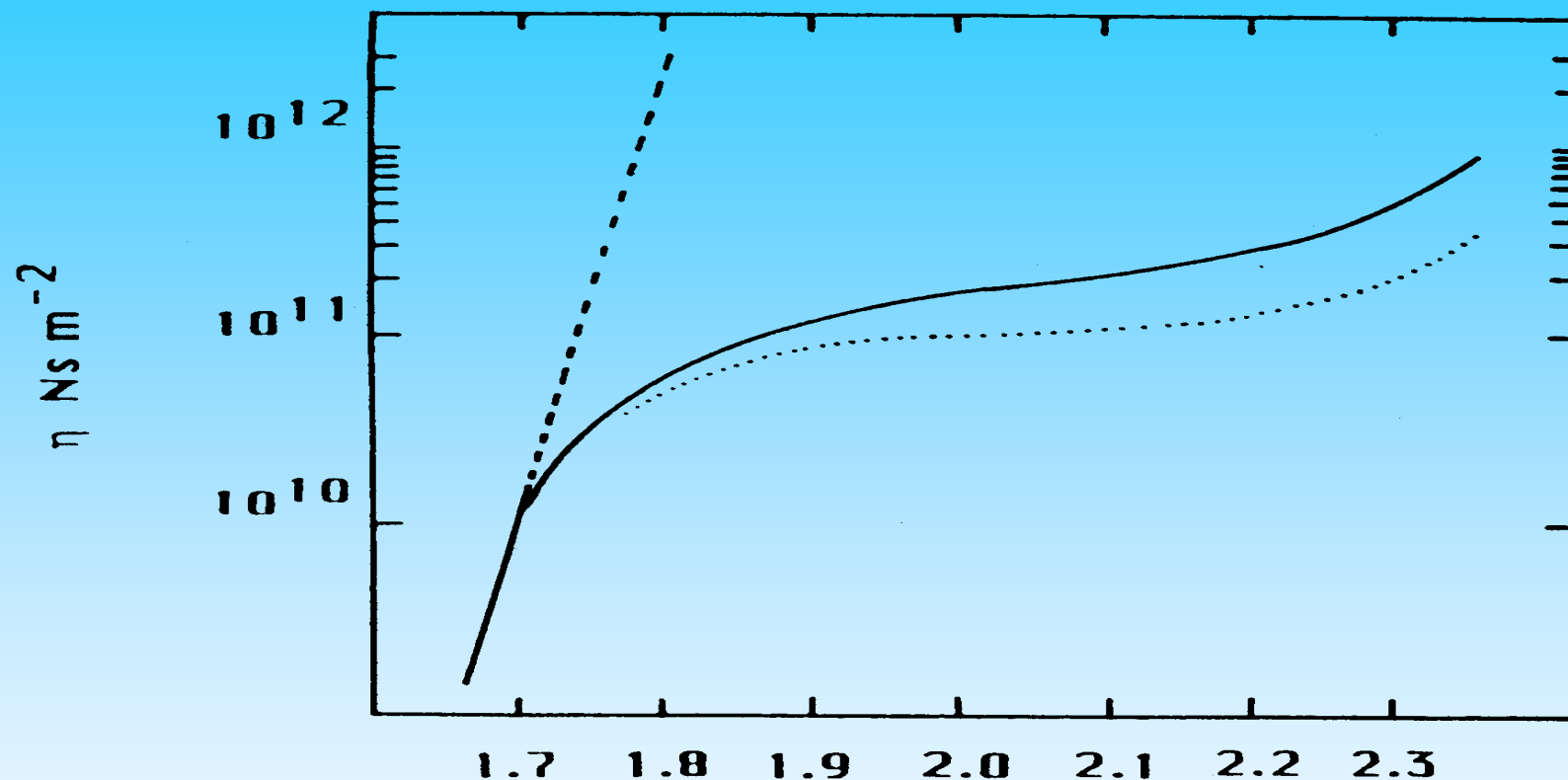
τ_{th} - the characteristic time for cooling of atomic subsystem

$$\tau_{th} \approx R_T^2 / D_a, (\tau_{th} \approx 10^{-11} - 10^{-9} \text{ s})$$

$$\tau_\sigma = \eta / \mu \leq \eta^* / \mu \approx \tau_{th} \approx R_T^2 / D_a$$

$$\mu \approx 100 \text{ GPa}, \eta^* \approx 1 - 100 \text{ Pas}$$

Viscosity behavior under irradiation

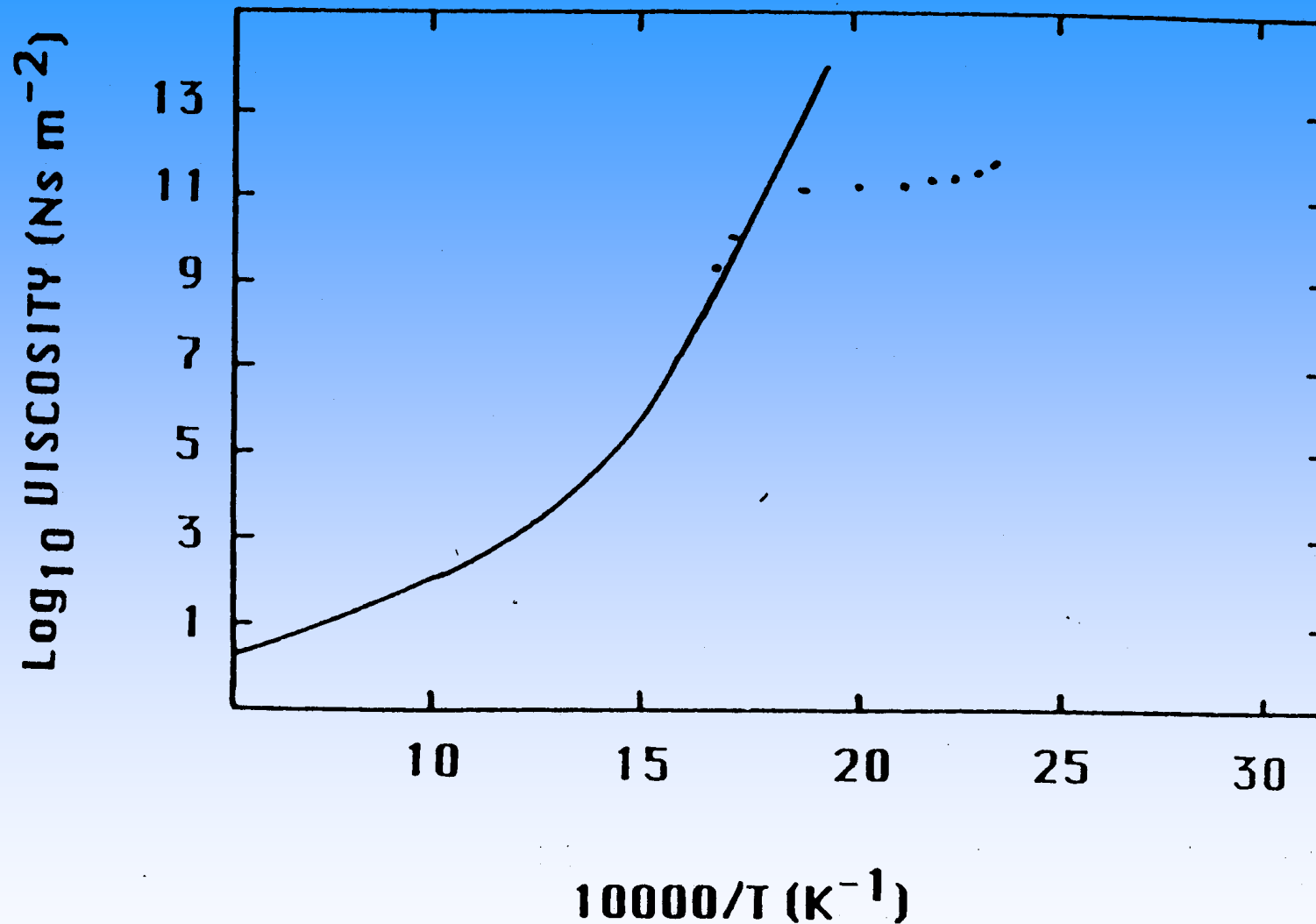


$1000/T$ (K^{-1}) B_2O_3 -glass fiber

Fig. 2. — — — Viscosity without irradiation, ———— viscosity under irradiation (experimental results), ······ viscosity under irradiation calculated for constant ions flux (correction made with the assumption that the viscosity is a linear function of the flux).

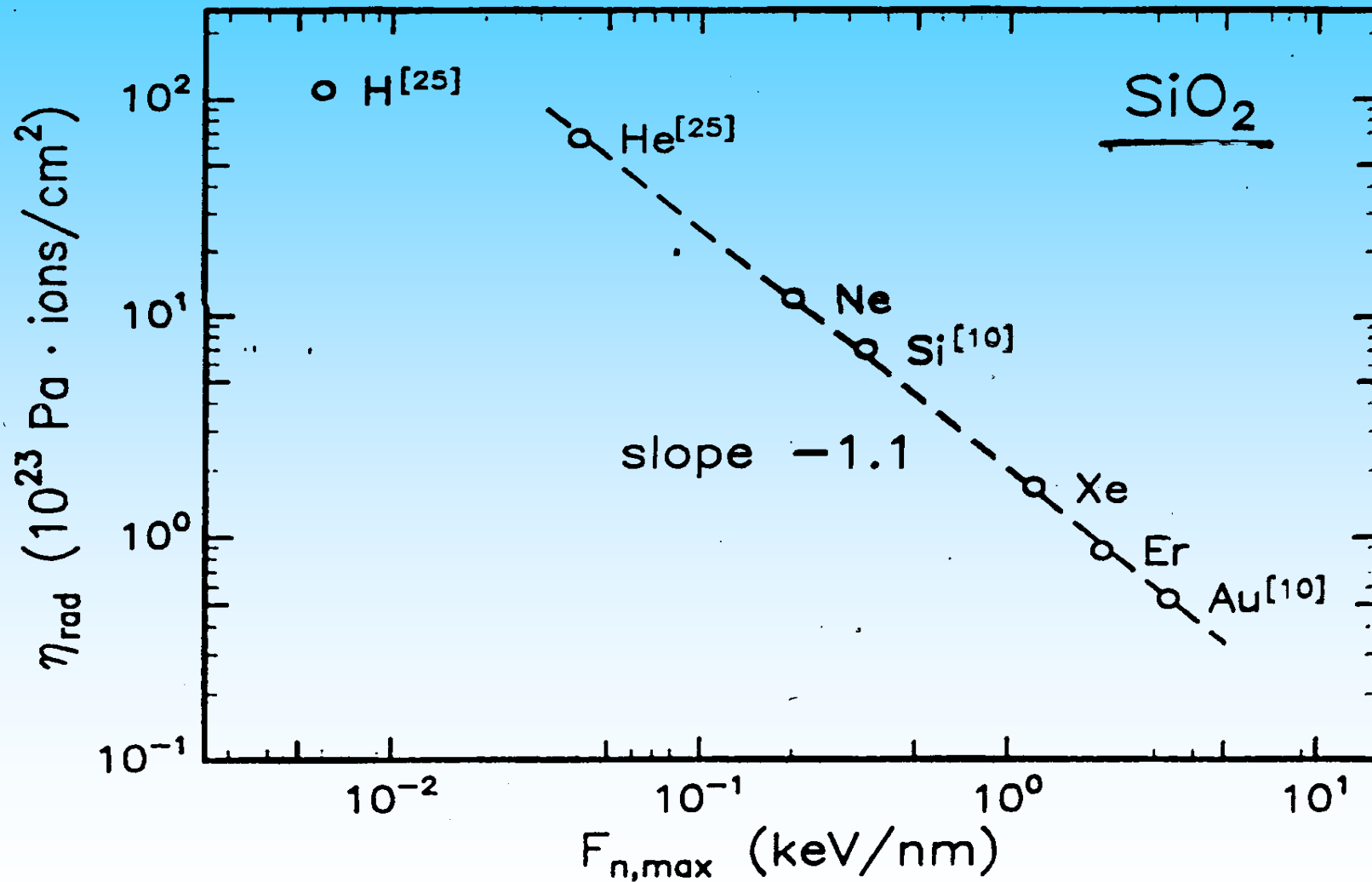
A.Burbu et.al.(1989) 13

Viscosity behavior under heavy ion irradiation



— Viscosity without irradiation, ······ viscosity under irradiation ($^{40}\text{Ar 44 MeV/R}$).

Radiation-induced viscosity as a function of deposited energy by elastic collisions



Radiation-enhanced viscous flow of irradiated amorphous alloys

Temperature dependence of viscosity of amorphous alloys

$$\frac{1}{\eta_{irr}} \propto \frac{n_f}{T_{irr}} \exp\left(-\frac{G}{T_{irr}}\right) \quad T_{irr} = T_0 + \Delta T_0(S_e)$$

- temperature of atoms in amorphous alloys (T_{irr})
- flow radiation defects (n_f), $n_f = \sigma_f(S_n, S_e)\Phi$
- new low activation energy (G)

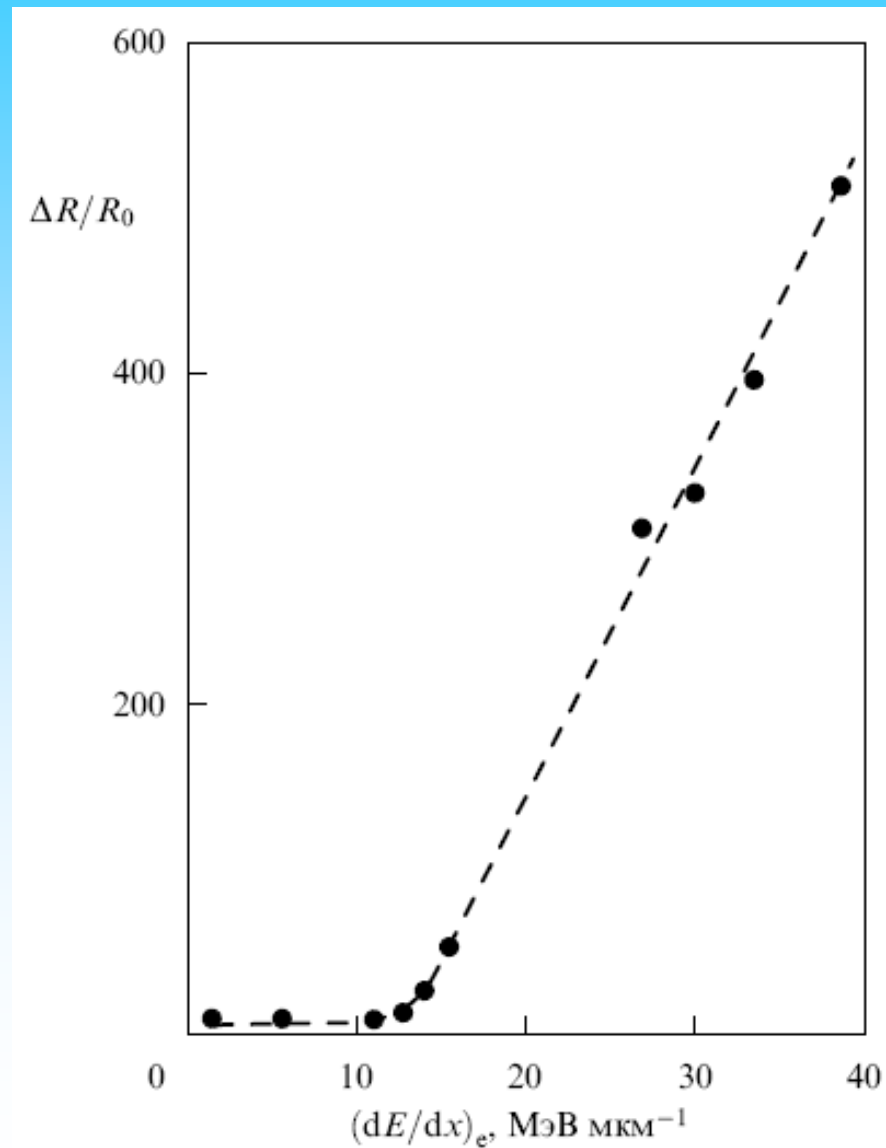
(Pd_{77.5} Cu₅ Si_{16.5} \longrightarrow after cold-rolling)

$G_0 = 2.0$ eV \longrightarrow $G_e = 0.4$ eV (S.S.Tsao, F.Spapen(1985))

$$\eta = \eta[n_f(\Phi_C), T_{irr}(S_e)] = \eta^*$$

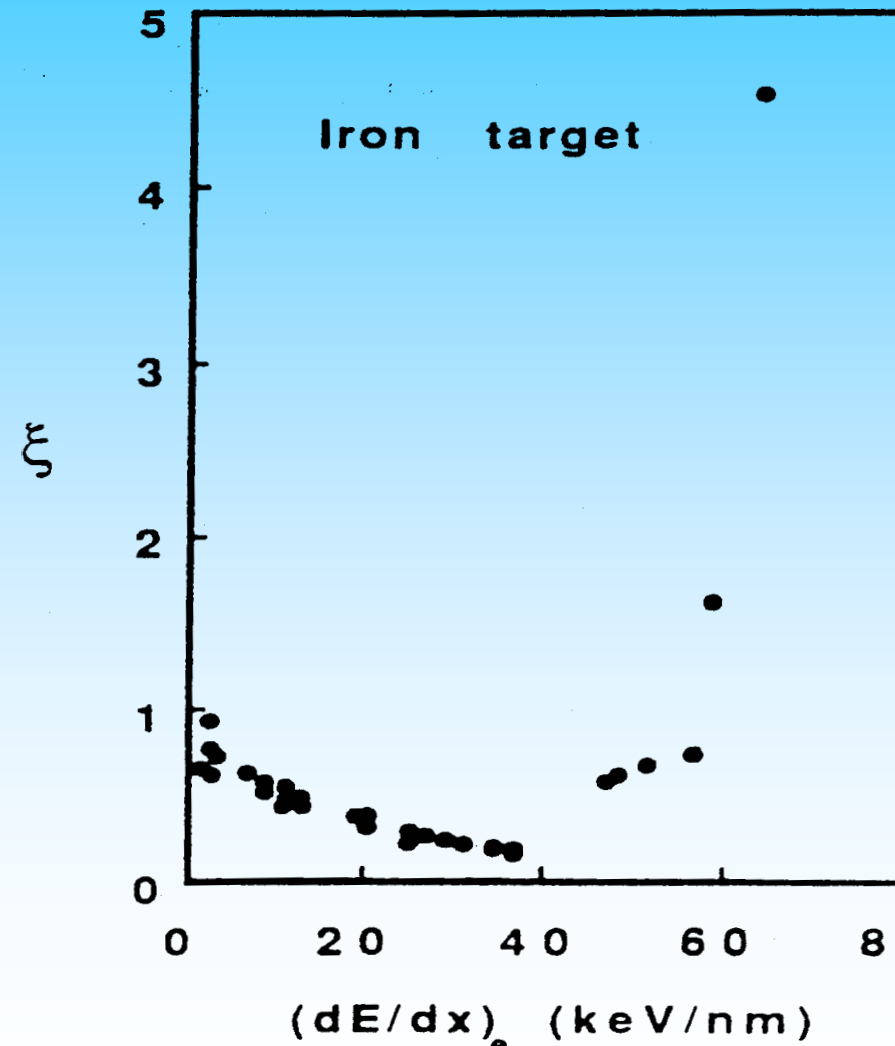
$$\Phi_C = \frac{B}{\sigma_f(S_e)} (T_n + S_e) \exp[G_n / (T_n + S_e)]$$

Dependence of electrical resistance of $\text{Fe}_{85}\text{B}_{15}$ from electronic losses of heavy ions



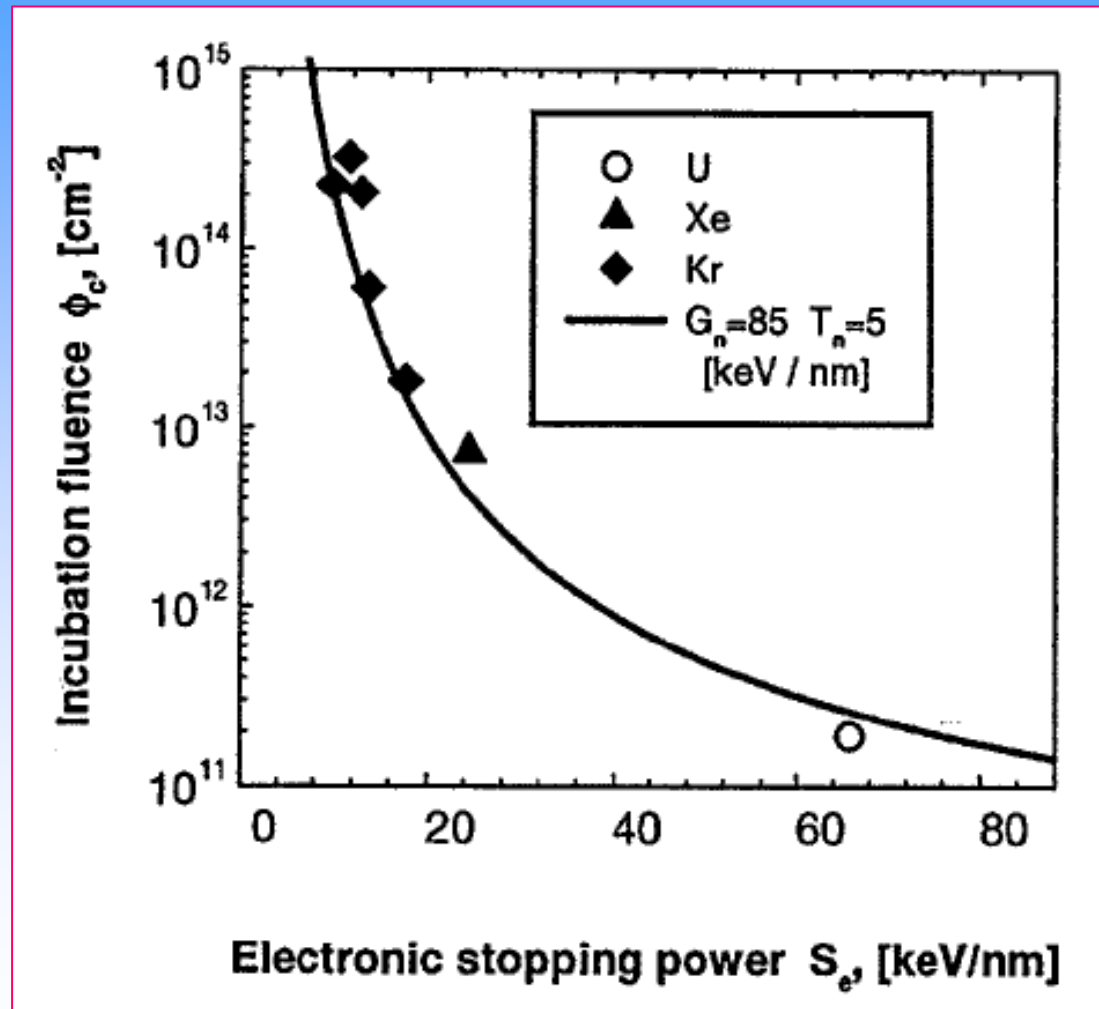
$T_{\text{irr}} = 90 \text{ K}$

Evolution of damage production efficiency in Fe as a function of deposited energy in electronic excitation



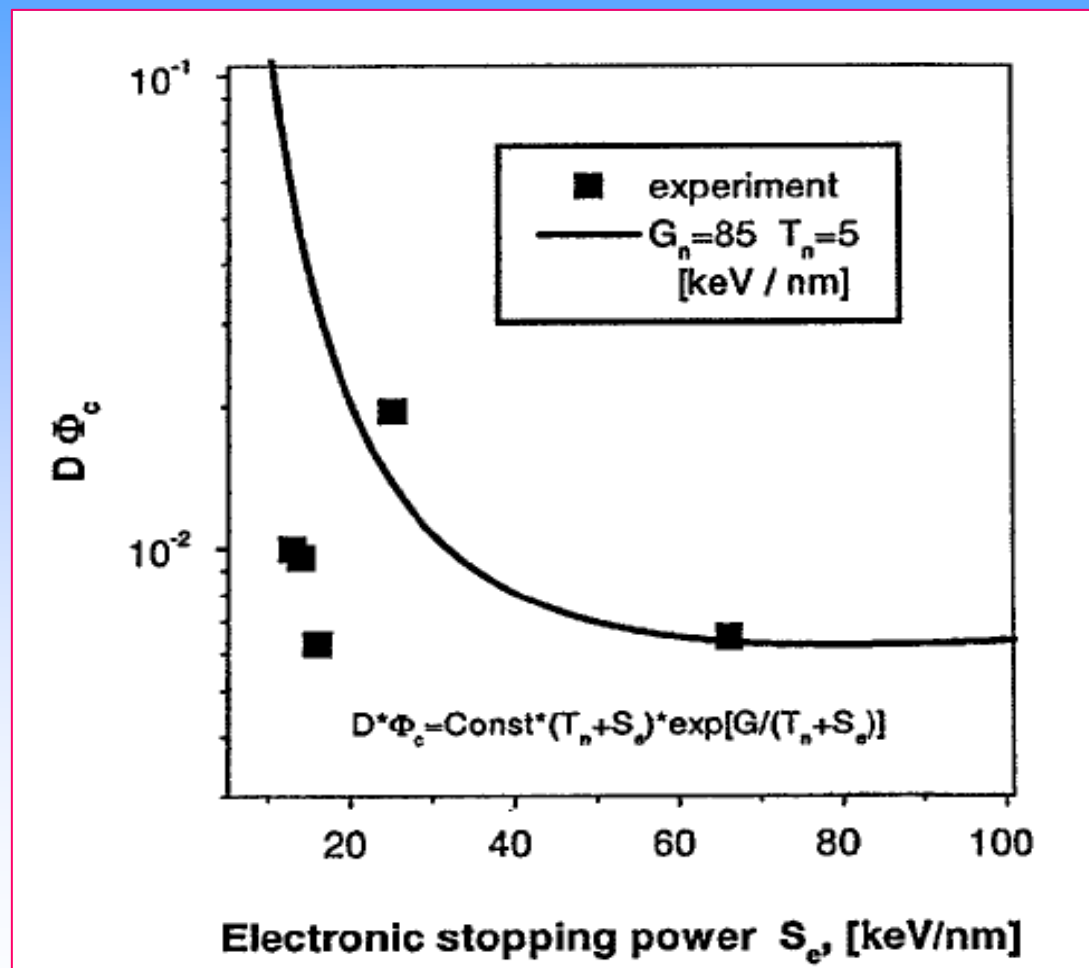
A. Dunlop et.al.(1989)

Dependence of the incubation fluence (Φ_c) on an electronic stopping power (S_e). The curve shows a fit to experimental data on the basis of developed theory.



A.I.Ryazanov, H.Trinkaus, A.E.Volkov , Phys.Rev.Lett.v.84 (2000) 919

Dependence of the incubation fluence (Φ_c) and the relative electrical resistance change at the beginning of an irradiation ($D = \sigma f \varphi$) on an electronic stopping power (S_e). The curve shows a fit to experimental data on the basis of developed theory.



A.I.Ryazanov, H.Trinkaus, A.E.Volkov , Phys.Rev.Lett.v.84 (2000) 919

Conclusion

- **The theoretical model of incubation dose for radiation growth of amorphous alloys is based on the viscoelastic behavior of these and drastic viscosity decrease after heavy ion irradiation.**
- **The developed theoretical model takes into account the effect of atomic displacements, ion temperature gradients arising due to interaction of an excited electronic subsystem with the ionic one.**
- **Incubation dose will disappear at sufficiently high electronic stopping power (S_e)**