

# **Radiation-induced softening vs. hardening effects in metals and alloys during simultaneous action of irradiation and mechanical strain**

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**"Materials resistant to extreme conditions for future energy systems".  
Kiev, Ukraine, 12-14 June 2017.**

# Content

## Radiation Induced Hardening (RIH)

- Pinning strength of defects : MD simulations
- Pinning strength of defects : experiment
- Kinetic theory of bridging MD with reality

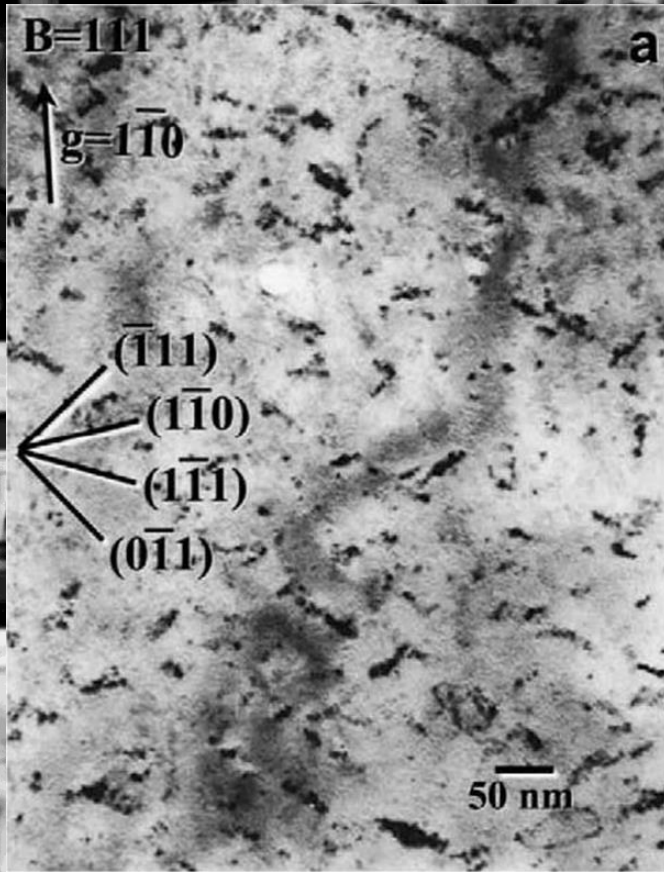
## Radiation Induced Softening (RIS)

- Experiment: in-reactor neutron irradiation
- Experiment: in-laboratory electron irradiation
- Theory: Localized Anharmonic Vibrations (LAV)
- Theory: LAV interaction with dislocations
- NP lifetime with account of both RIH and RIS

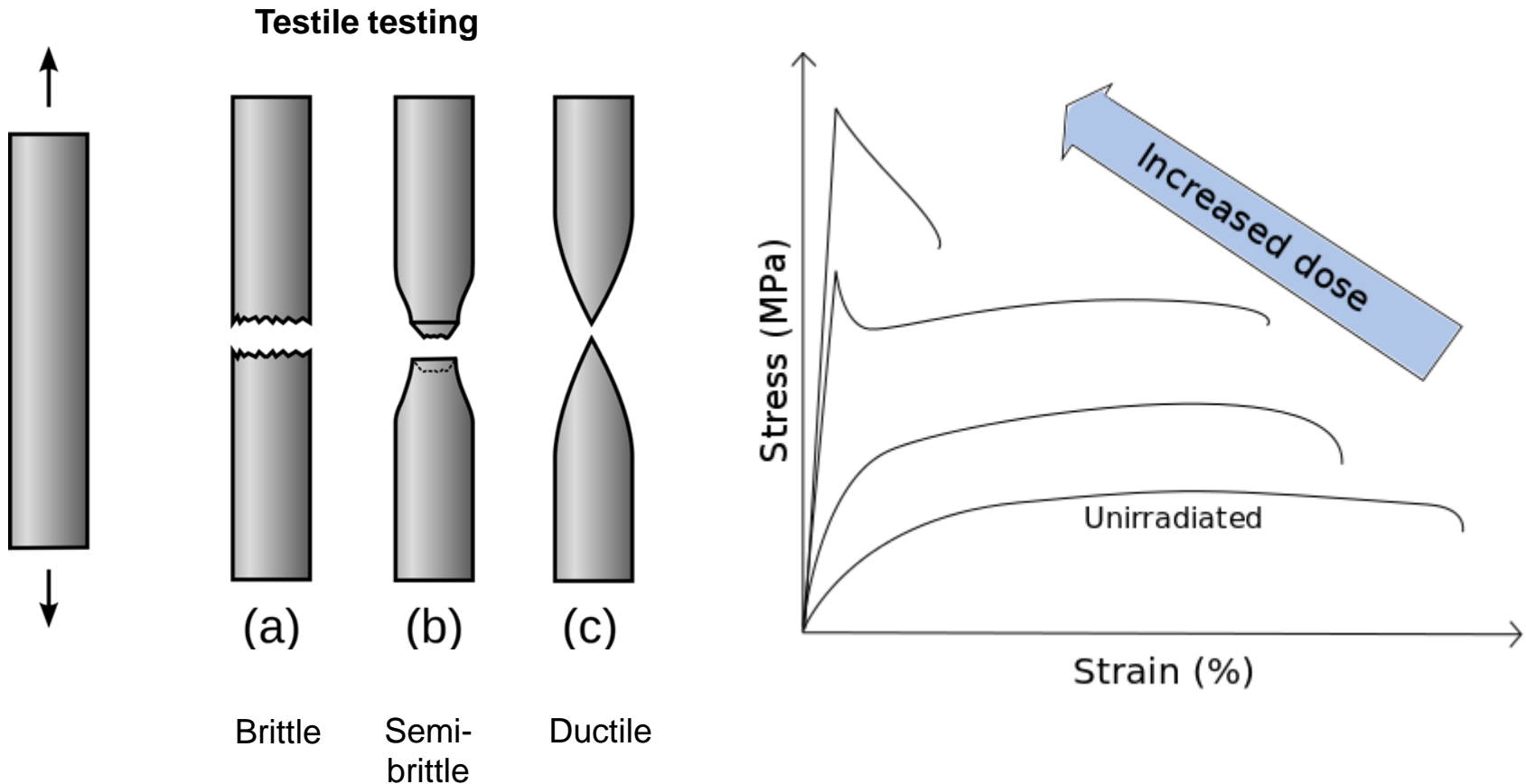
## Conclusions and Outlook

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OCT. 10, 1956

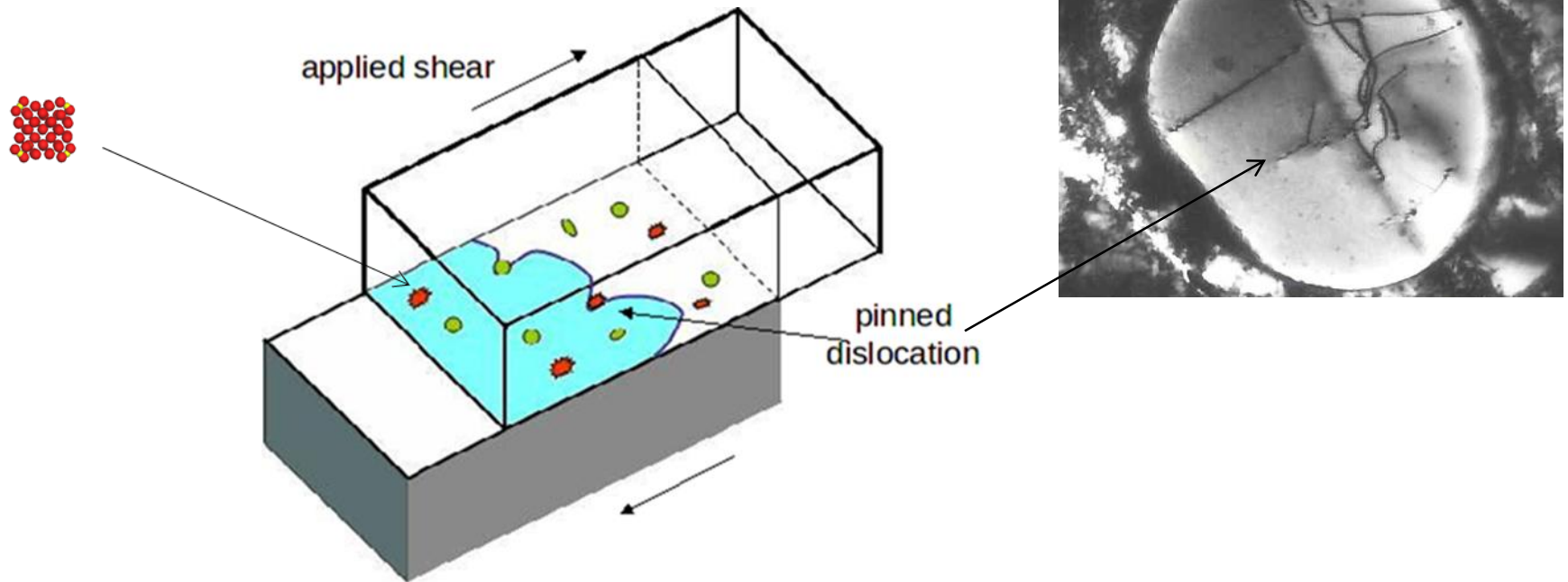


# Macroscopic impact: Embrittlement



Mobility of dislocations keeps the steel ductile

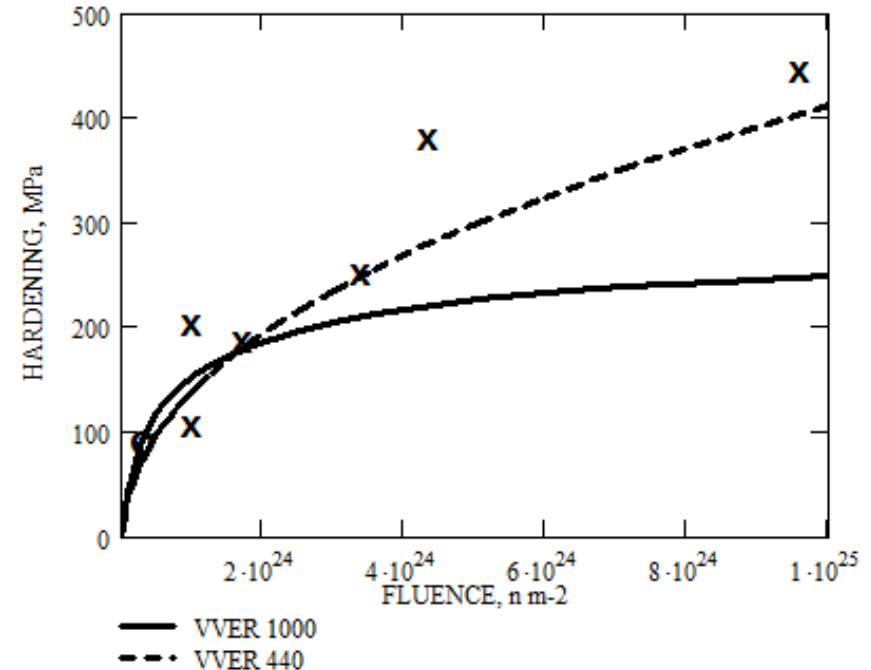
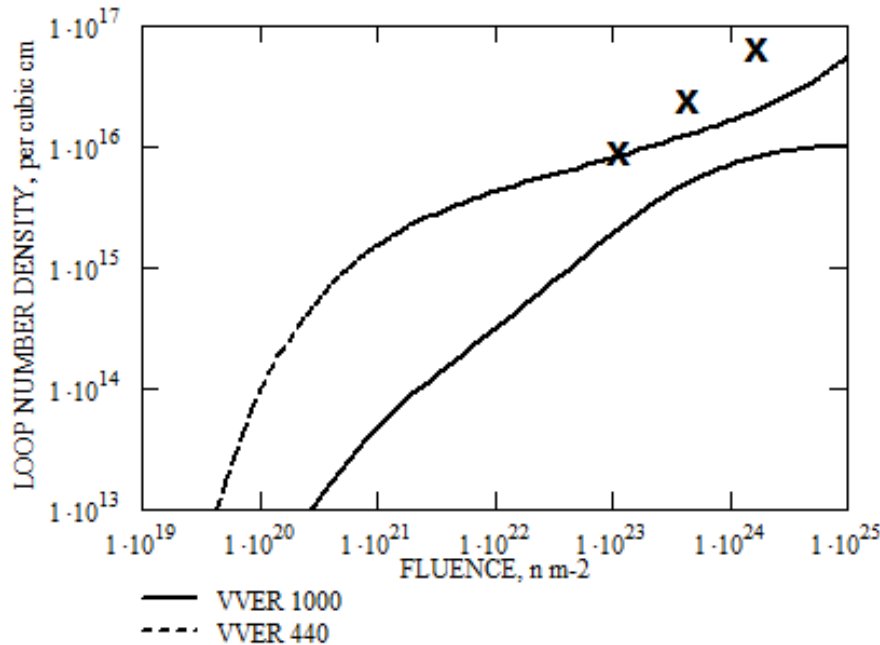
# Dislocations



Point defects, such as SIA and vacancies, hinder the movements of dislocations

# IRRADIATION HARDENING OF REACTOR PRESSURE VESSEL STEELS DUE TO THE DISLOCATION LOOP EVOLUTION

V. I. Dubinko, S. A. Kotrechko, V. F. Klepikov, *Radiat. Eff.* 2009



Dependence of the total loop number density and loop-induced hardening on the neutron fluence vs. experimental data for WWER-440 and WWER-1000,  $T_{irr} = 300$  °C; (o) - experimental data for PVS steel 15K h2NMFA in WWER-1000; (x) – experimental data for 15Kh2MFA irradiated in WWER-440

# Temperature dependence of irradiation hardening due to dislocation loops and precipitates in RPV steels and model alloys

S. Kotrechko, V. Dubinko, N. Stetsenko, D. Terentyev, Xinfu He, M. Sorokin

J. Nucl. Mater. (2015)

$$\Delta\sigma_Y = \alpha Gb\sqrt{N \times d}$$

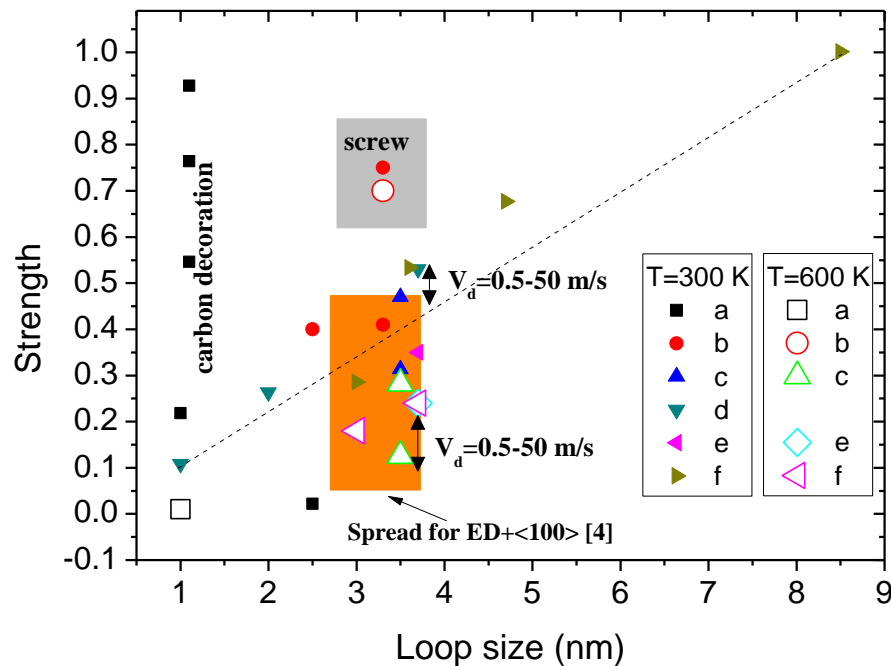
$$\alpha = \alpha_0 \cdot 0.465 \ln\left(\frac{1}{2b\sqrt{N \times d}}\right)$$

$$\Delta\sigma_Y = \Delta\sigma_{Y1} + \Delta\sigma_{Y2}$$

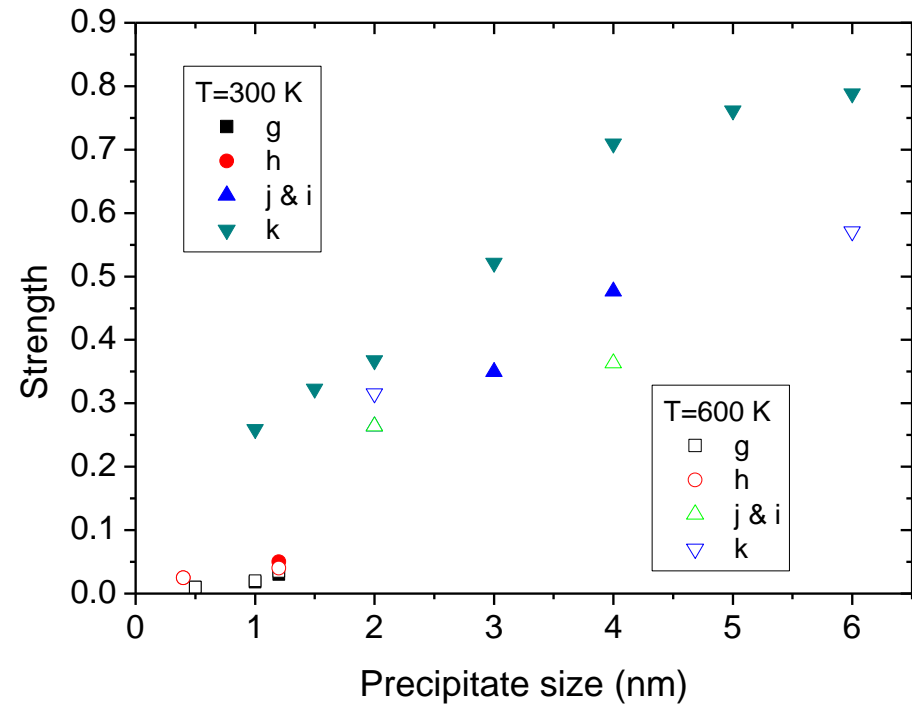
Linear superposition

# MD simulation results on pinning strength of DL and precipitates

## DL



## Precipitates



Strain Rate  $\sim 10^7 \text{ s}^{-1}$  (!!!)



Kotrechko, Dubinko et al (2015)

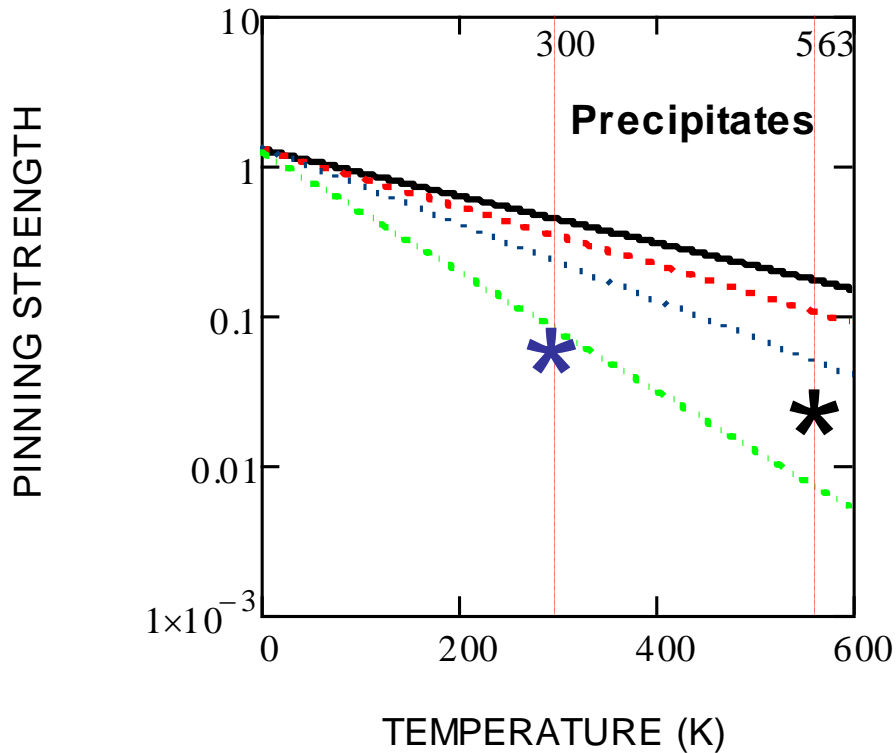
**Temperature dependence of the pinning strength:**

$$\alpha_i(T) = 0.85M \frac{F}{2\pi} \ln \left( \frac{1}{2b\sqrt{N_{irr} \times d_{irr}}} \right) \alpha_{0,i}(T)$$

$$\alpha_{0,i}(T) = \alpha_{0,i}(0) \exp \left\{ -\beta_i T \right\}$$

$$\beta_i = \frac{k_B \ln(\dot{\epsilon}_0 / \dot{\epsilon})}{U_{0,i}}$$

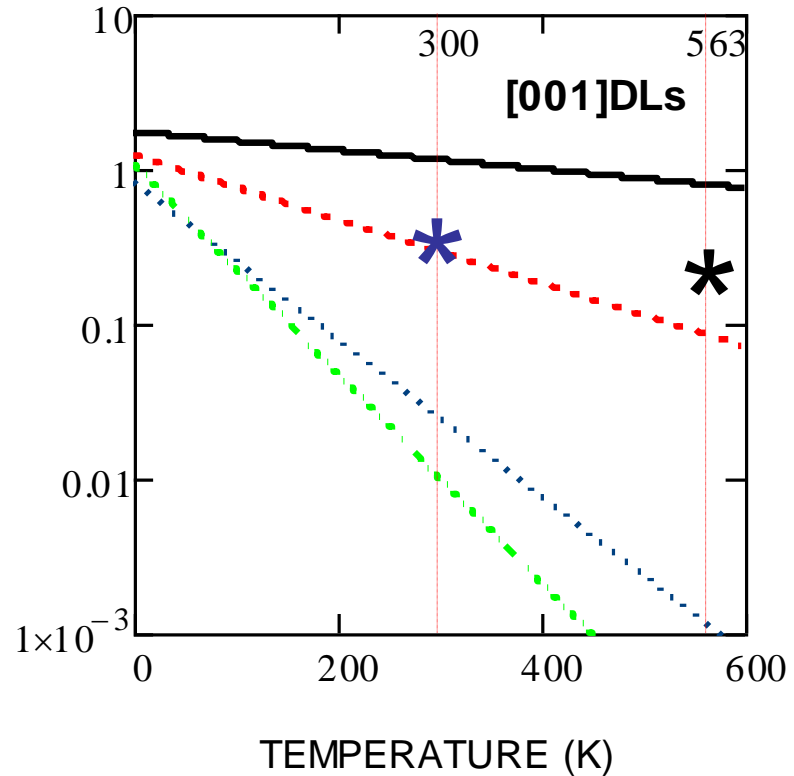
# Temperature dependence of pinning strength at experimental strain rate $10^{-4} \text{ s}^{-1}$



- 6 nm
- - - 5 nm
- ... 4 nm
- · - 3 nm

Experiment

- \* Western
- \* Russian



- 7.2 nm
- - - 3.7 nm
- ... 2.6 nm
- · - 1.7 nm

# **RADIATION-INDUCED SOFTENING (RIS-effect)**

# Conventional view

Mechanical properties are determined by microstructure ( $U_0$ ), temperature ( $T$ ) strain rate  $\dot{\epsilon}$

$$\Delta\sigma_Y(T) \approx \sum_i \sigma_{th,i}^{irr}(T) \quad \sigma_{th,i}^{irr}(T) = \alpha_{irr,i}(T) Gb \sqrt{N_{irr,i} \times d_{irr,i}}$$

$$\alpha_{irr,i}(T) = 0.85M \frac{F}{2\pi} \ln \left( \frac{1}{2b\sqrt{N_{irr,i} \times d_{irr,i}}} \right) \alpha_{0,i}^{irr}(T)$$

$$\alpha_{0,i}^{irr}(T) = \alpha_{0,i}^{irr}(0) \exp \left\{ -\beta_i^{irr} T \right\}$$

$$\beta^{irr} = \frac{k \ln(\dot{\epsilon}_0 / \dot{\epsilon})}{U_0^{irr}}$$

# Present theory

Mechanical properties are determined **additionally** by the irradiation flux  $F$

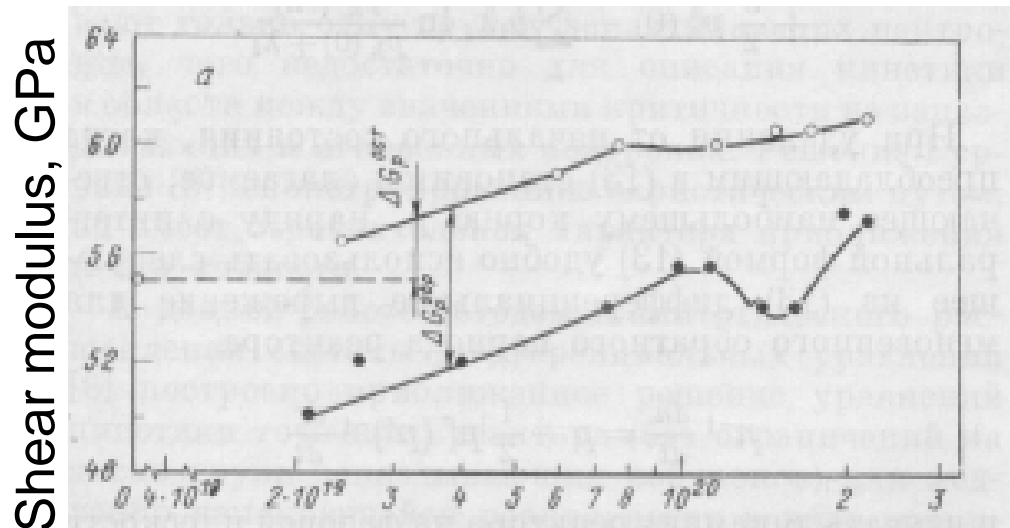
$$\beta_L^F(F) = \frac{k \ln \left( \frac{\dot{\varepsilon}_0}{\dot{\varepsilon}} \left( 1 + I_0 \left( \frac{E_{ex}}{k_b T} \right) \omega_{ex}(F) \tau_{ex} \right) \right)}{U_{0,L}^{irr}}$$

## In-reactor tests:

### Reversible decrease of the shear modulus of iron and its alloys under irradiation

Grynik, Karasev, Atomnaya Energiya 54 (1983) 177 (in Russian)

Institute for Nuclear Research, Kiev, Ukraine



Dependence of *shear modulus* in Fe on fast neutron fluence ( $E > 0.1 \text{ MeV}, 10^{14} \text{ n/cm}^2\text{s}$ ) at  $580 \text{ }^\circ\text{C}$  under *in-situ* irradiation (●) and after reactor was stopped (○).

Fluence ( $\text{n/cm}^2$ )

$$\Delta G_{irr} = \Delta G_{irr}^{residual} - \Delta G_{irr}^{reversible} < 0$$

Similar reversible effects was observed in the earlier works by Grynik and Karsev for Ni and Fe-<sup>11</sup>B in 1973-83

**Technological significance of these results is as follows.**

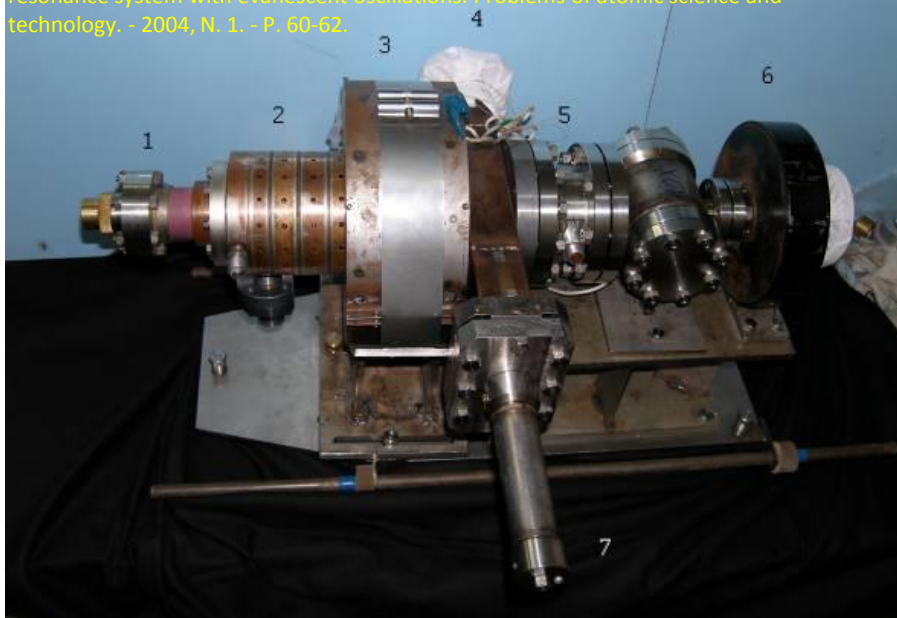
**It is known that mechanical testing is done using the so called "surveillance specimens" irradiated prior to the mechanical testing. However, the results from INR have demonstrated unambiguously that mechanical properties of materials under irradiation may differ significantly from those after irradiation.**

We have tested some metals including **Cu, Al, Zr, St. steel** under in-situ electron irradiation, both sub-and over-threshold and demonstrated similar Radiation-Induced Softening (RIS) effect in all cases under investigation.

# Experimental investigation of the electron-plastic effect under electron irradiation

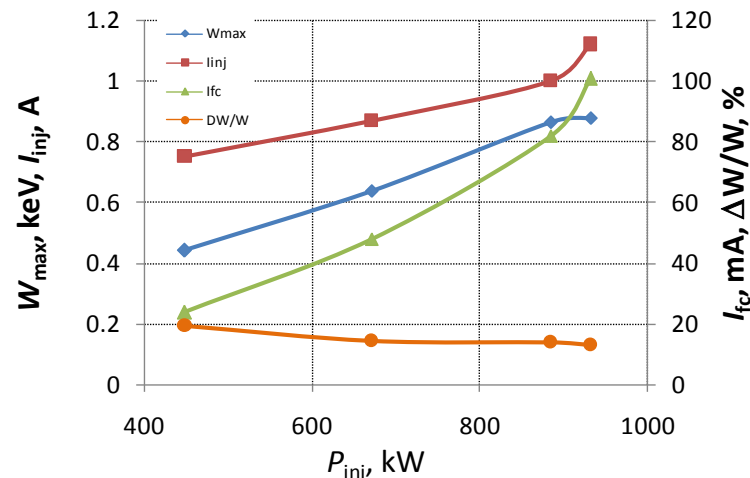
## Kushnir, Lebedev et al, NSC KIPT, 2008

\* M.I. Ayzatsky, E.Z. Bifer, N.G. Golovko et al. Electron injector based on resonance system with evanescent oscillations. Problems of atomic science and technology. - 2004, N. 1. - P. 60-62.



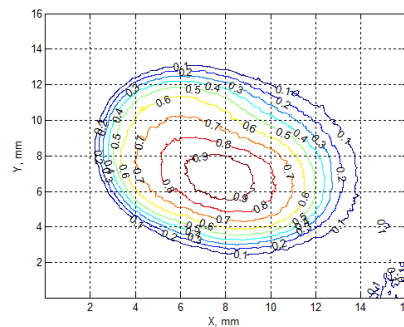
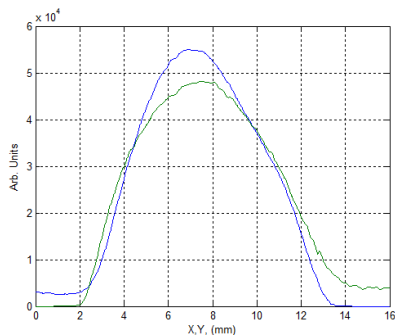
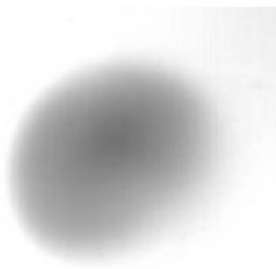
Инжектор в сборе: 1 – катодный узел электронной пушки, 2 – группирователь, 3 – соленоид, 4 – подводящий волновод, 5 – датчик тока пучка, 6 – магнитная линза, 7 – механизм перемещения короткозамкнутого поршня

### Диапазон основных параметров пучка в зависимости от мощности СВЧ питания



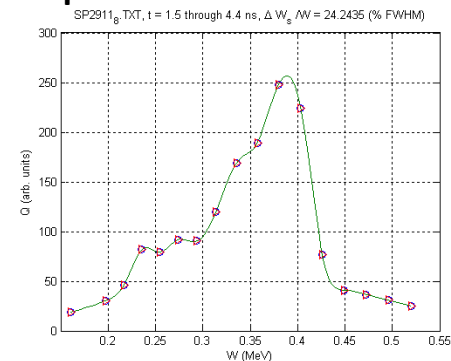
$W_{max}$  – энергия электронов на выходе источника,  
 $I_{inj}$  – ток пучка электронов на выходе источника,  
 $I_{fc}$  – ток пучка электронов в плоскости мишени,  
 $\Delta W/W$  – ширина энергетического спектра

### Отпечаток пучка в плоскости мишени



$\Delta X = 7.9492$  mm,  $\Delta Y = 7.0343$  mm (на уровне половинной интенсивности)

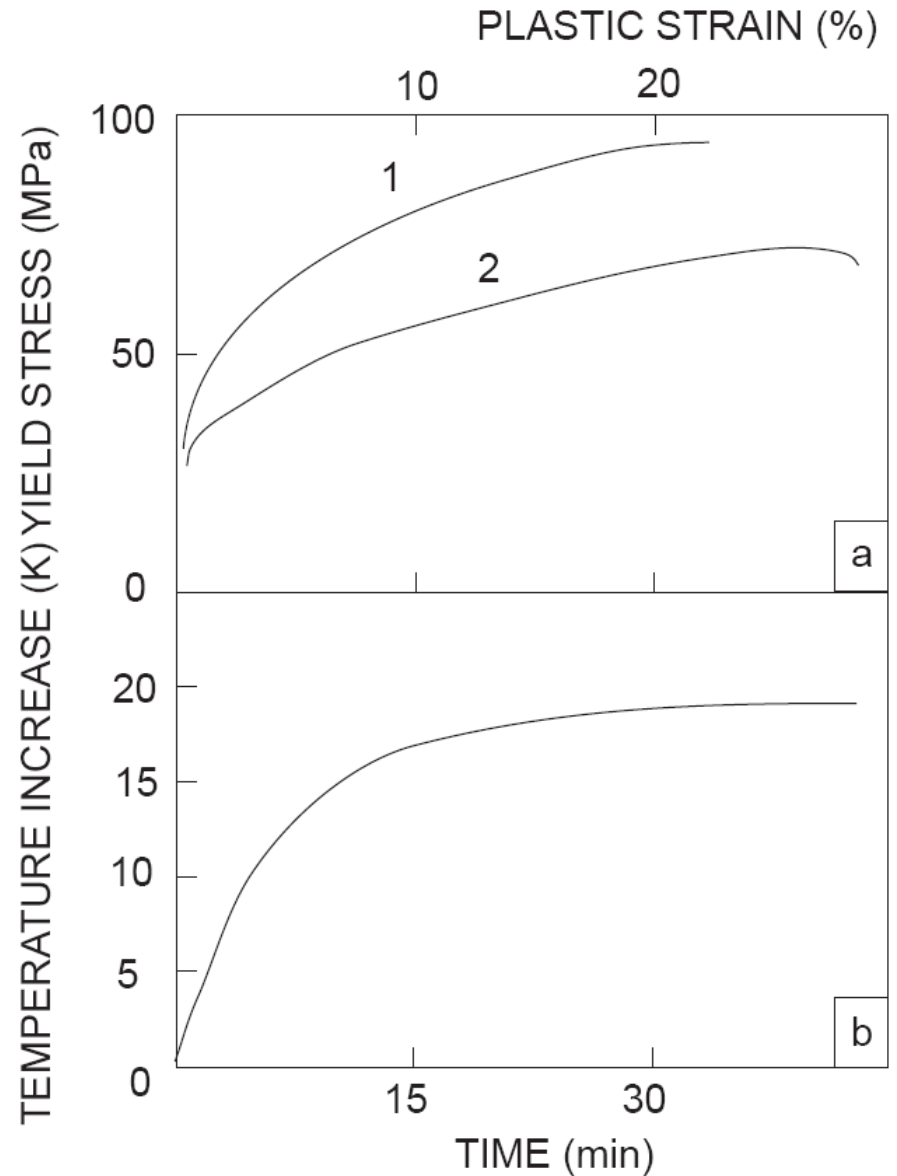
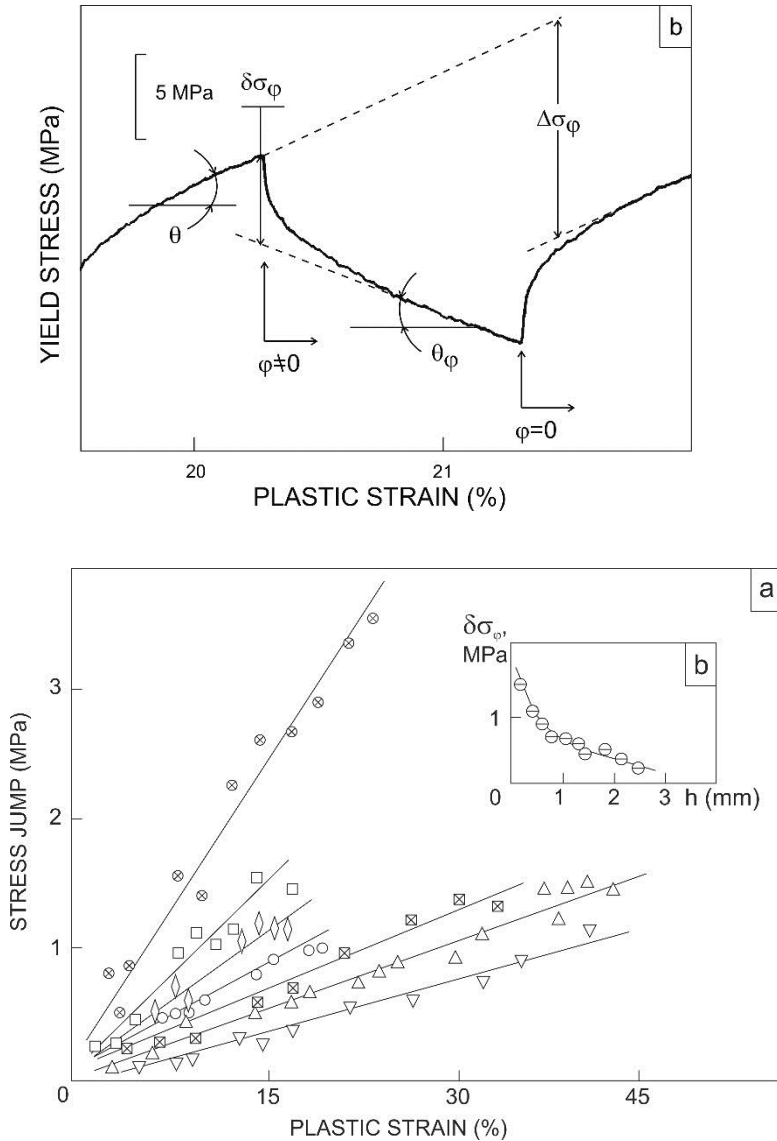
### Распределение электронов по энергиям в плоскости мишени



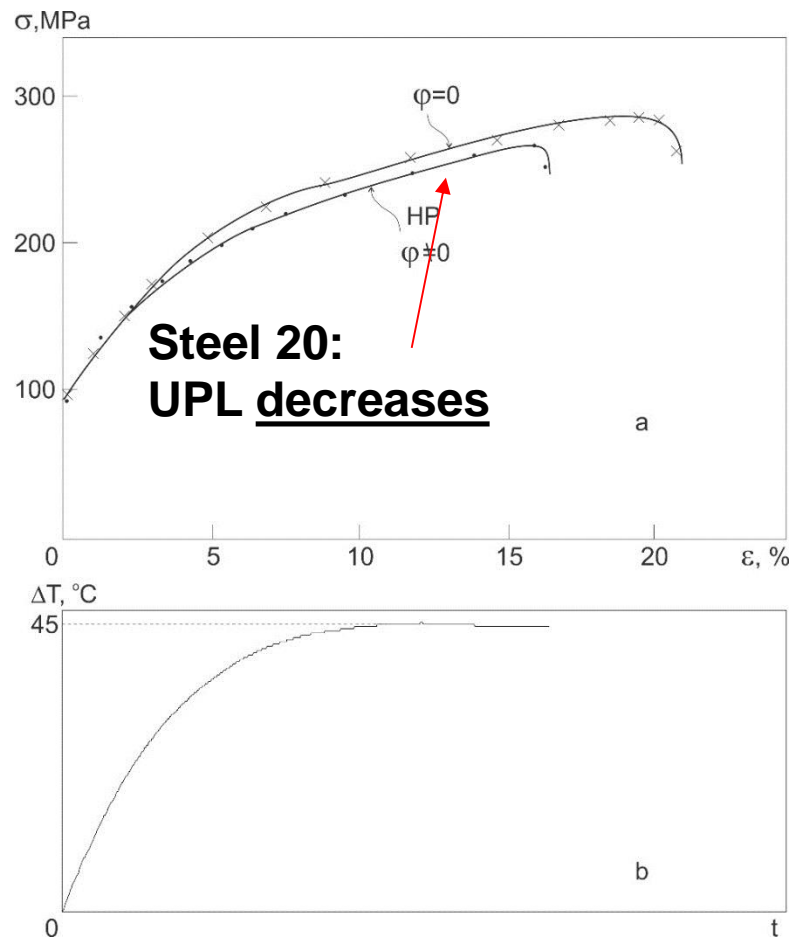
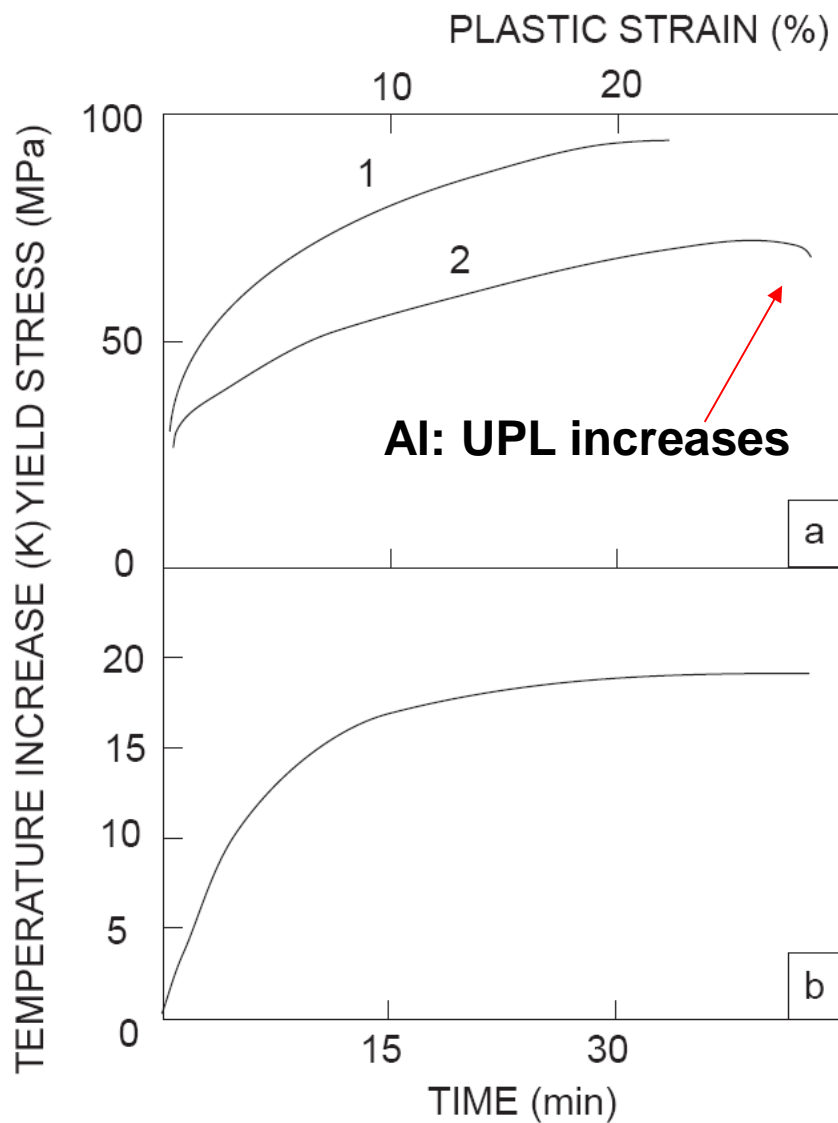
$W_{max} = 390$  keV,  $\Delta W/W = 24\%$  (FWHM)



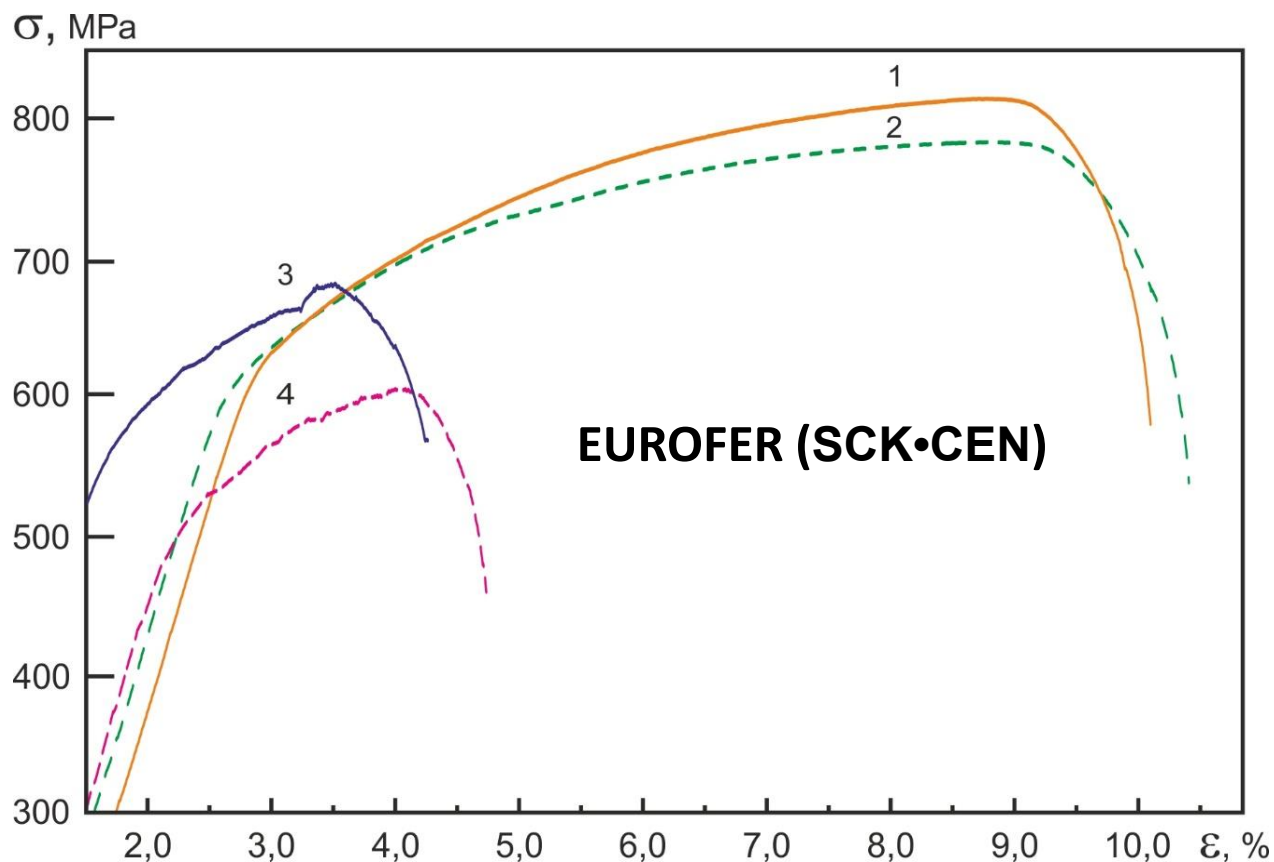
# Radiation-Induced Softening: experiment (Al)



# Ultimate plasticity limit (UPL) under continuous 0.5 MeV electron irradiation of Al and Fe at the electron flux of $\sim 10^{18} \text{ m}^{-2} \text{ s}^{-1}$ (dose rate of $10^{-9} \text{ s}^{-1}$ )



Euro fer	Composition, wt%																
	C	N	Al	Si	P	S	Ti	V	Cr	Mn	Ni	Cu	As	Nb	Mo	Sn	W
T91	0.10	0.04	0.01	0.22	0.02	0.00	0.00	0.21	8.99	0.38	0.11	0.06	0.00	0.06	0.89	0.00	0.01
		42	5		1	04	3						8			4	



**Deformation curve for reactor steel T91 (EUROFER) without irradiation (1, 3) and at  $\varphi = 4.0 \cdot 10^{16} \text{ m}^{-2} \cdot \text{s}^{-1}$  (2);  $1.9 \cdot 10^{16} \text{ m}^{-2} \cdot \text{s}^{-1}$  (4) at RT (1, 2) and at 553 K (3, 4)**

# Theory of RIS:

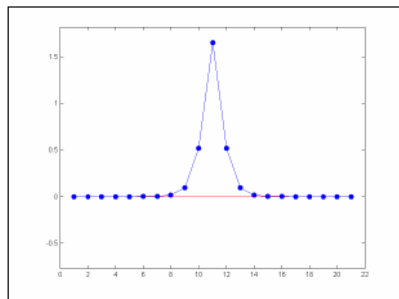
Irradiation produces Localized Anharmonic Vibrations (**LAV**) that assist the unpinning of dislocations from nanometric precipitates and dislocation loops

## Nonlinear coupled oscillators



$$V = \sum V(X_n) + C W(X_n, X_{n+1})$$

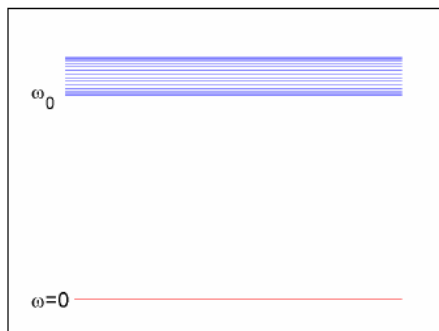
- Exact, periodic and localized solution



The concept of **LAV** in regular lattices is based on *large anharmonic* atomic oscillations in **Discrete Breathers** excited **outside the phonon bands**.

## Phonons

- Frequency band  $\omega_{ph}^2 = \omega_0^2 + 4C \sin^2 q/2$
- Non localized states

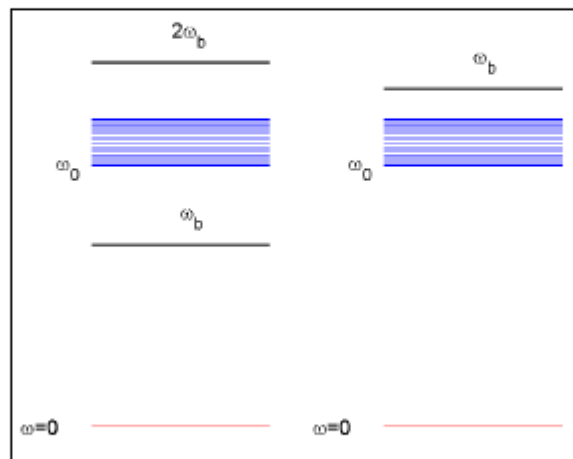


## Existence of breathers (1994)



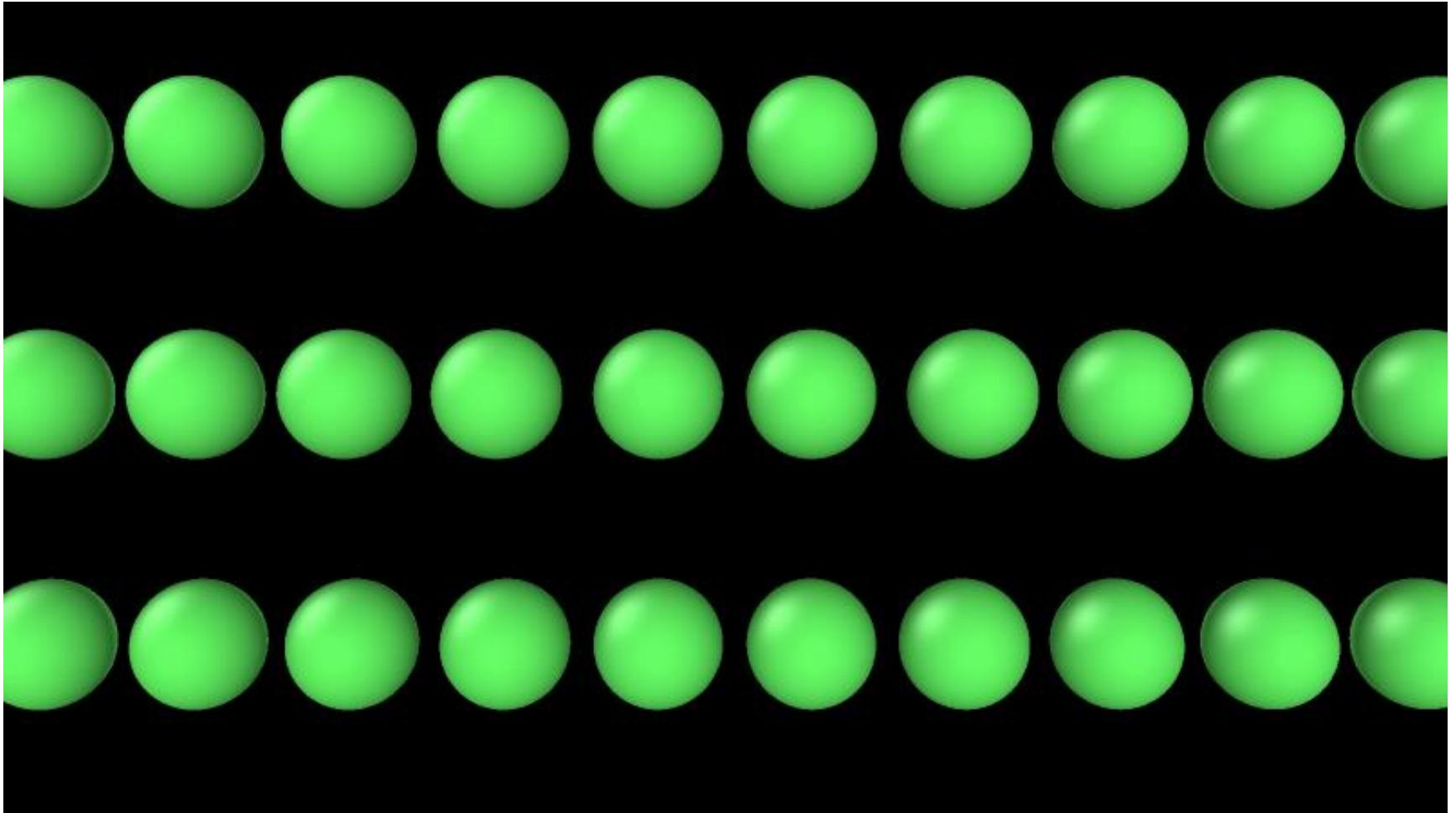
Soft

Hard



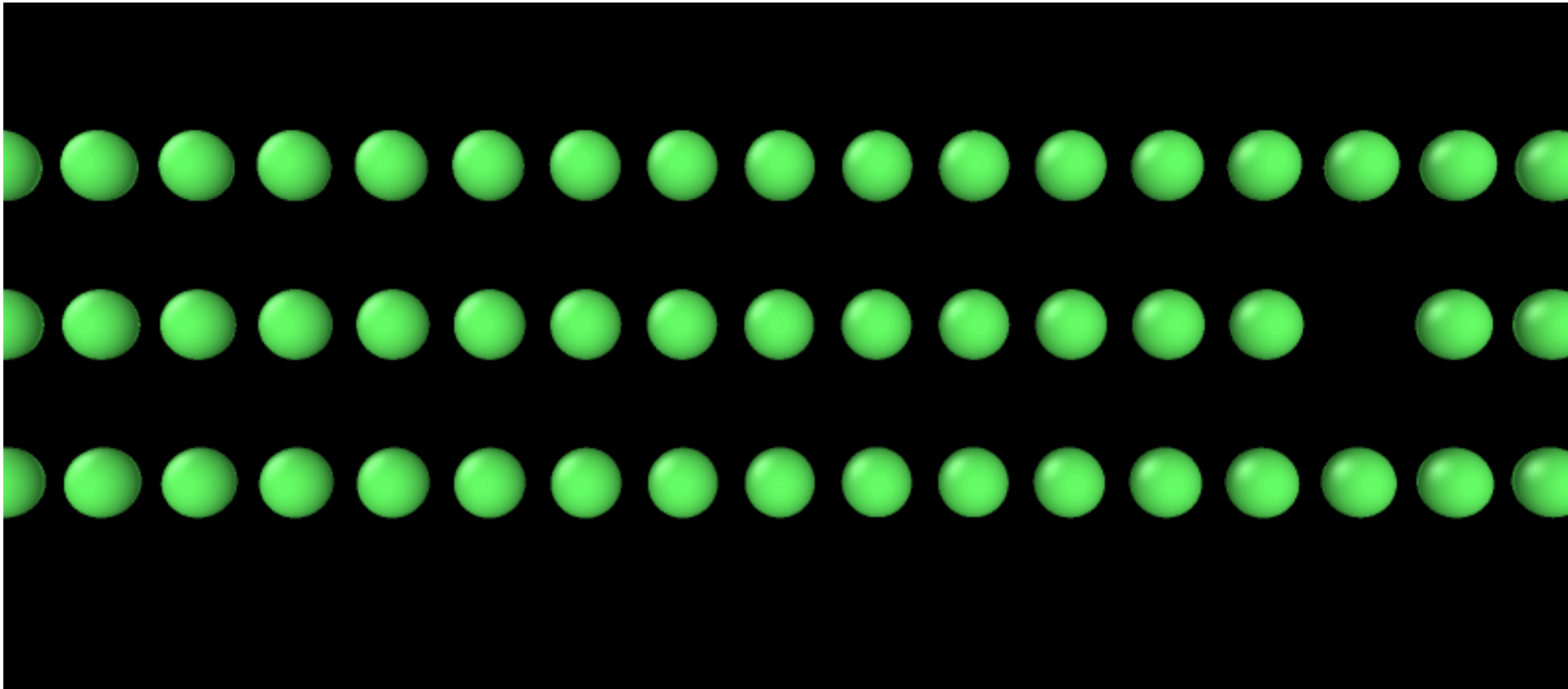
$$\exists \omega_b \notin [\omega_0, \omega_{f,\max}], \quad \omega_b'(E) \neq 0$$

**Standing DB in bcc Fe:  $d_0=0.3 \text{ \AA}$**   
D.Terentyev, V. Dubinko, A. Dubinko (2013)



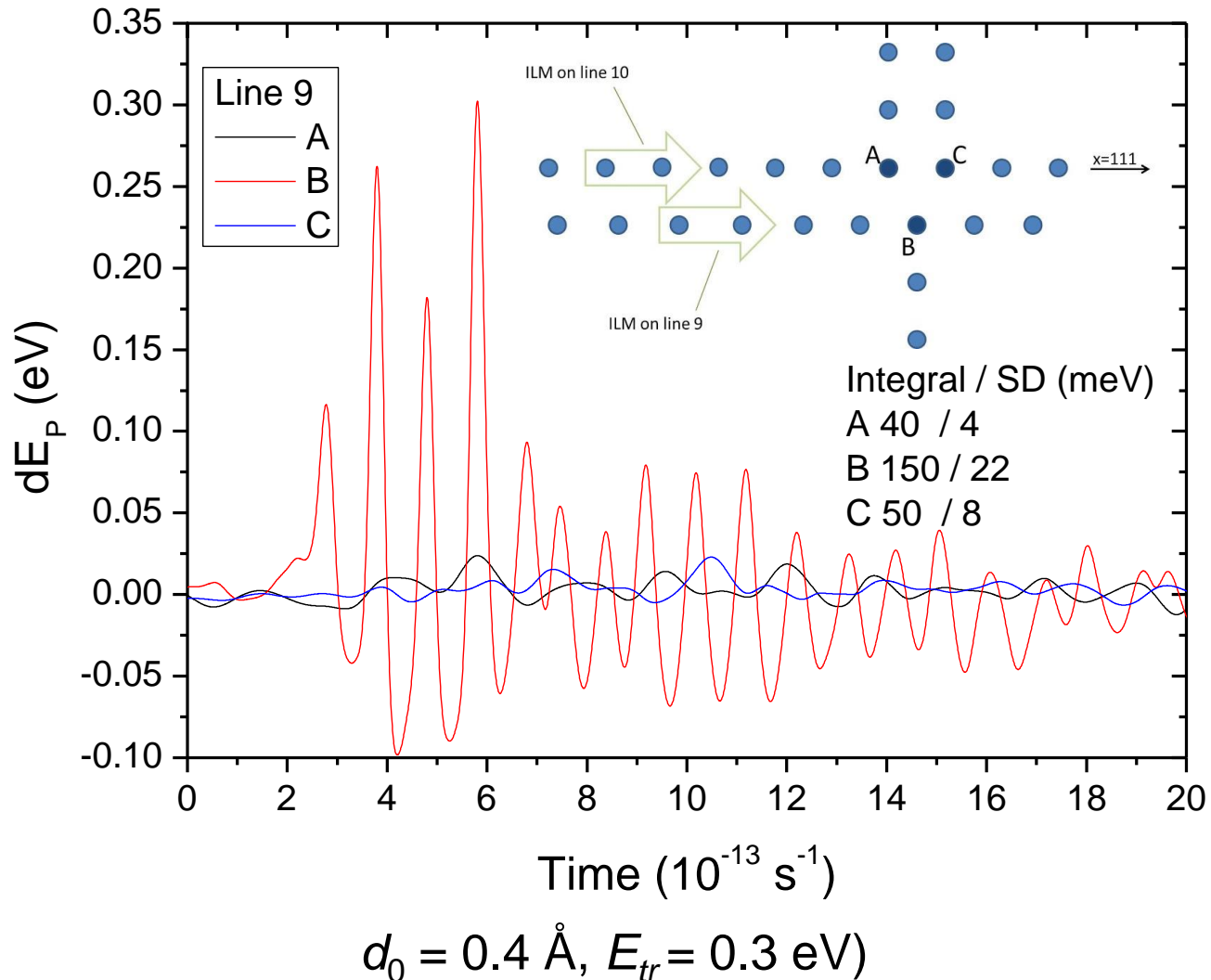
# Moving DB in bcc Fe: $d_0=0.4 \text{ \AA}$ , $E=0.3 \text{ eV}$

D.Terentyev, V. Dubinko, A. Dubinko (2013)



# Interaction of discrete breathers with primary lattice defects in bcc Fe

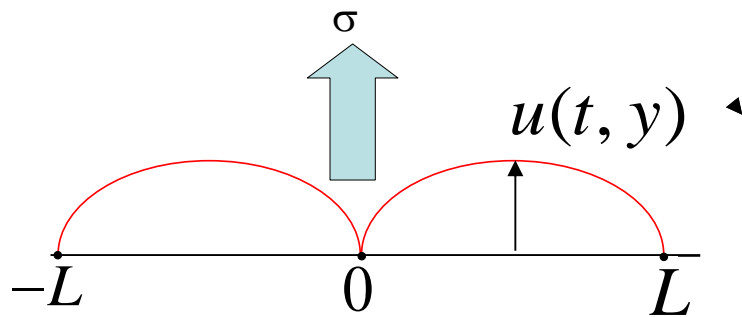
Terentyev, Dubinko et al, *Modelling Simul. Mater. Sci. Eng.* **23** (2015)





# String model of the dislocation segment oscillations

A.I. Landau, Yu.I. Gofman, 1974



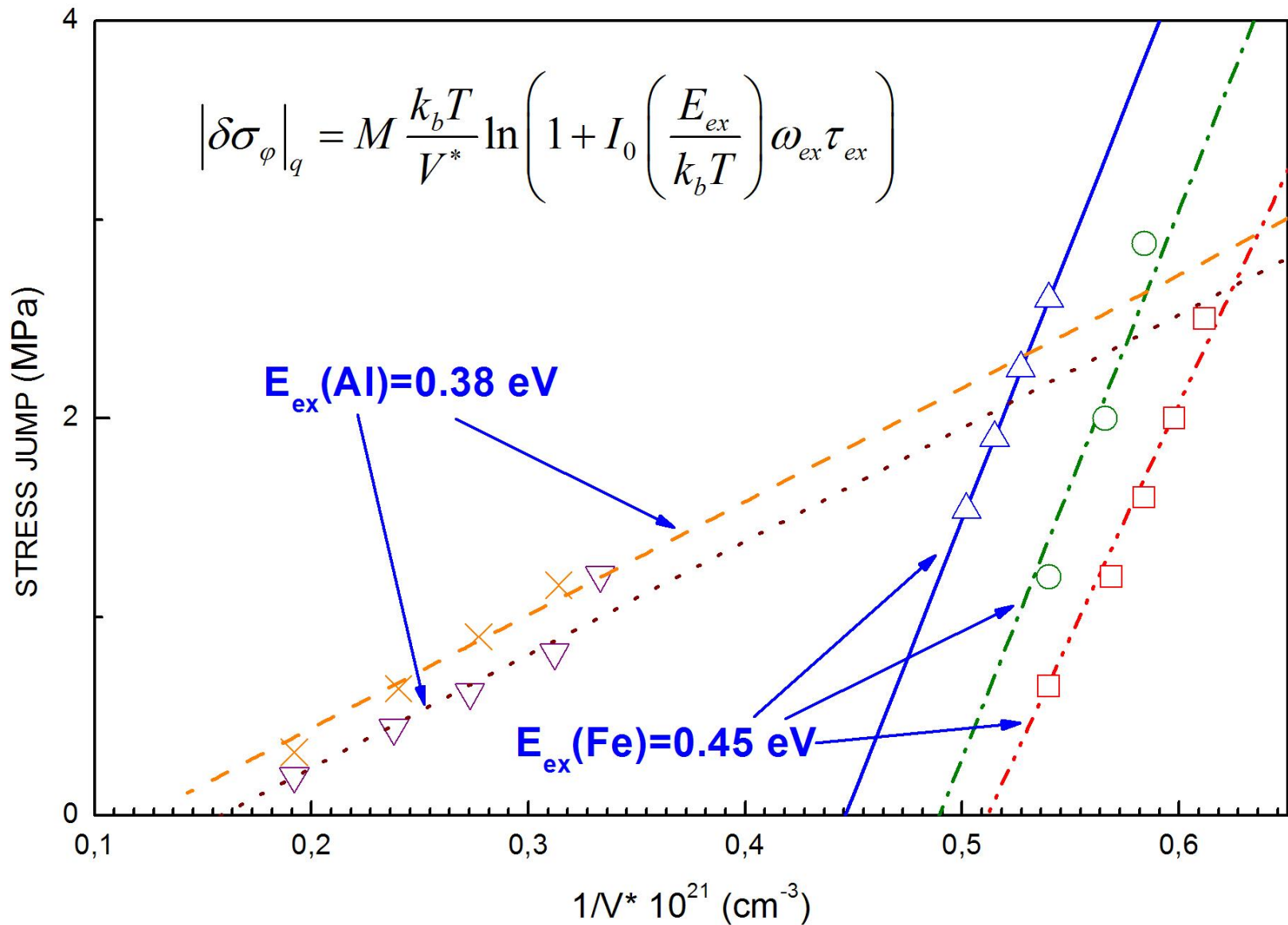
$$M \frac{\partial^2 u}{\partial t^2} + B \frac{\partial u}{\partial t} - C \frac{\partial^2 u}{\partial y^2} = b\sigma + f(t)$$

$$U(x) = \begin{cases} \zeta x^2, & |x| \leq x_{kp} \\ 0, & |x| > x_{kp} \end{cases} \quad \zeta x_{kp}^2 = U_0$$

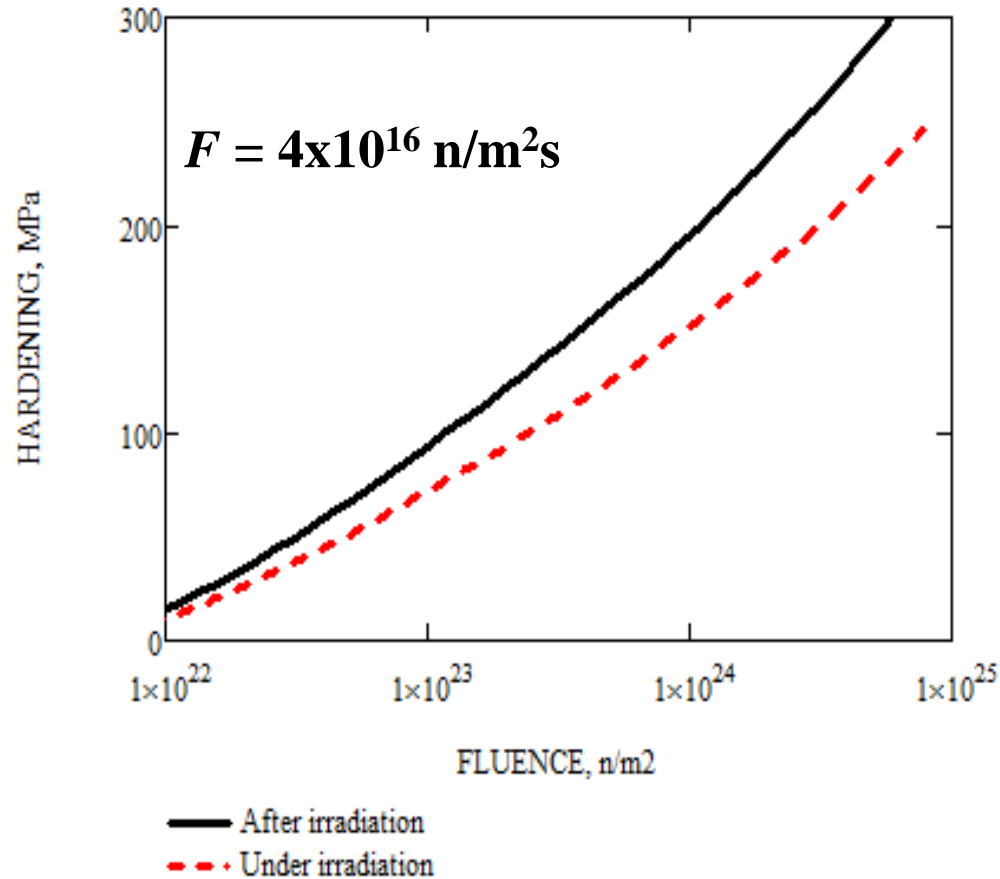
$$u'_y(0, t) = \kappa u(0, t) \quad -u'_y(L, t) = \kappa u(L, t) \quad \kappa = \frac{2\zeta}{C}$$

$f(t)$  Arbitrary force acting on dislocation- due to thermal vibration of atoms and radiation-induced LAVs!

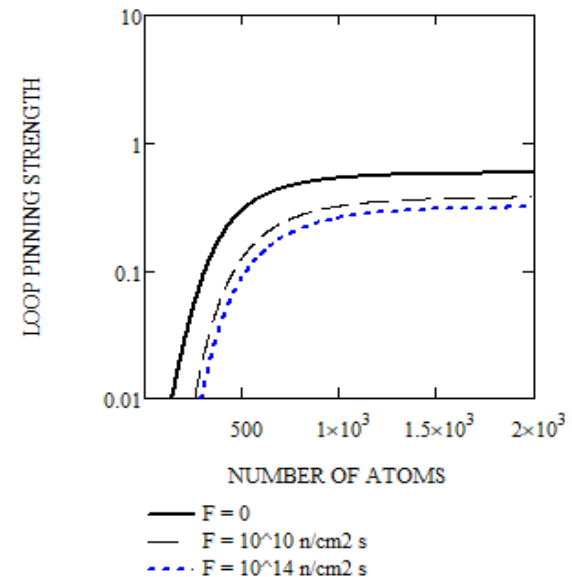
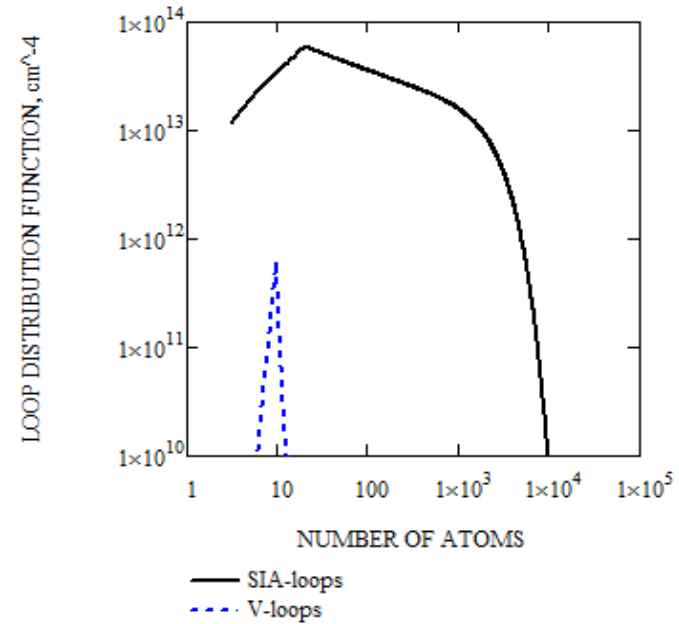
# Radiation-Induced Softening: model



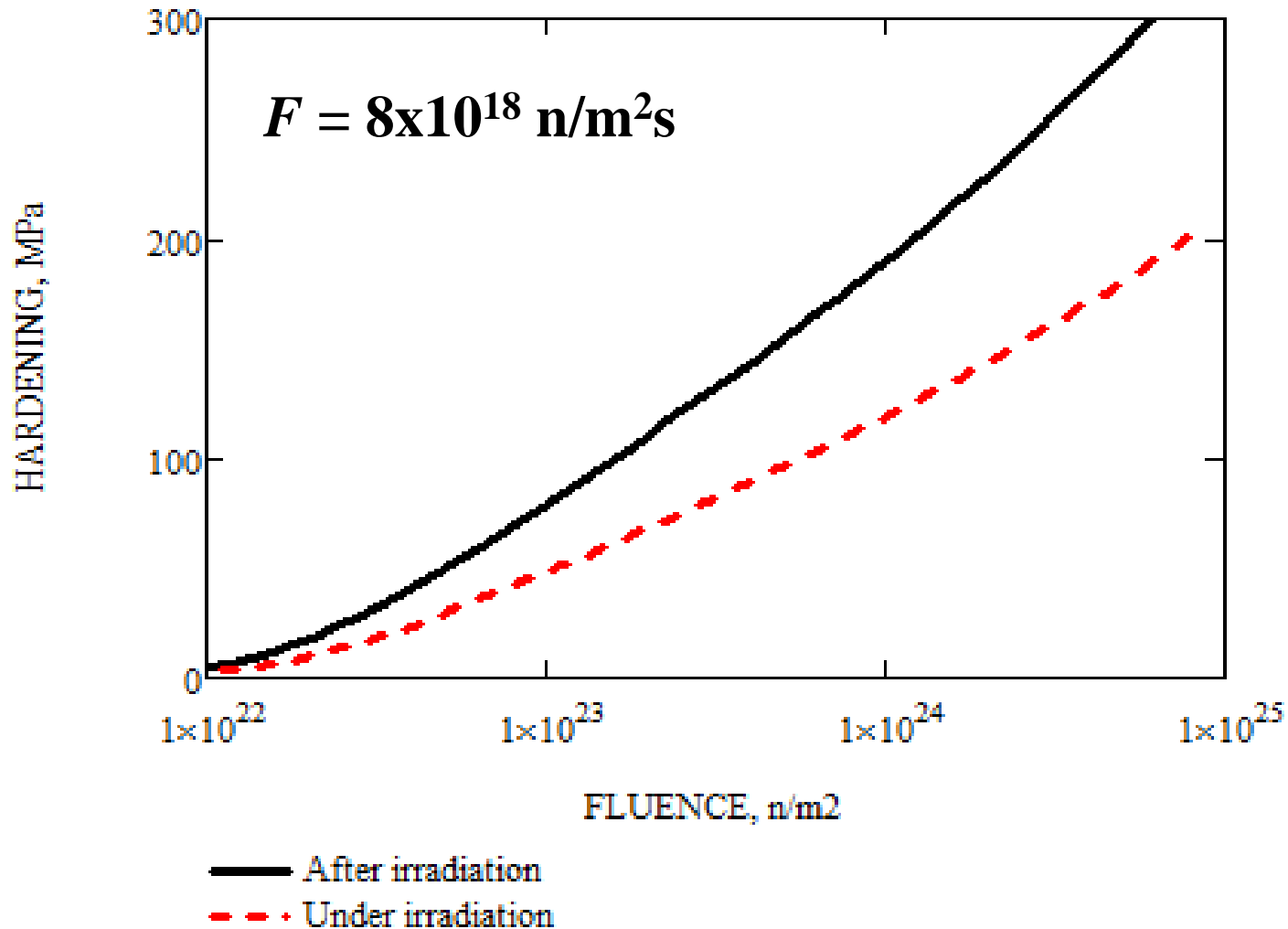
# The calculated hardening of Fe due to dislocation loop formation *under* different neutron fluxes compared to the hardening *after* irradiation



$$\beta_L^F(F) = \frac{k \ln \left( \frac{\dot{\epsilon}_0}{\dot{\epsilon}} \left( 1 + I_0 \left( \frac{E_{ex}}{k_b T} \right) \omega_{ex}(F) \tau_{ex} \right) \right)}{U_{0,L}^{irr}}$$



The calculated hardening of Fe due to dislocation loop formation *under* different neutron fluxes compared to the hardening *after* irradiation



# Conclusions and outlook

- Pinning strength of radiation-induced nanometric defects strongly depends on **strain rate**, **temperature** and **irradiation flux** (**RIS effect**)
- Experimental facility** for mechanical testing of nuclear materials under ***in situ* reactor irradiation** is extremely expensive and time-consuming
- We in Kharkov, have a unique (so far) installation for testing mechanical properties of nuclear materials under *in-situ* electron irradiation, which can be used as a pilot launch for more costly and time-consuming in-reactor testing.
- Compact *neutron source* is under construction

**Neutron source with *neutron energy* 2.5 MeV and *flux*  $3 \times 10^9$  n/s  
'Accelerator' R&D Establishment NSC KIPT**



**THANK YOU  
FOR YOUR ATTENTION!**