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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

Modeling of radiation effects in vanadium

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Effect of Solute Atoms on Microstructure Changes in Irradiated Binary Vanadium Alloys

A.I. Ryazanov

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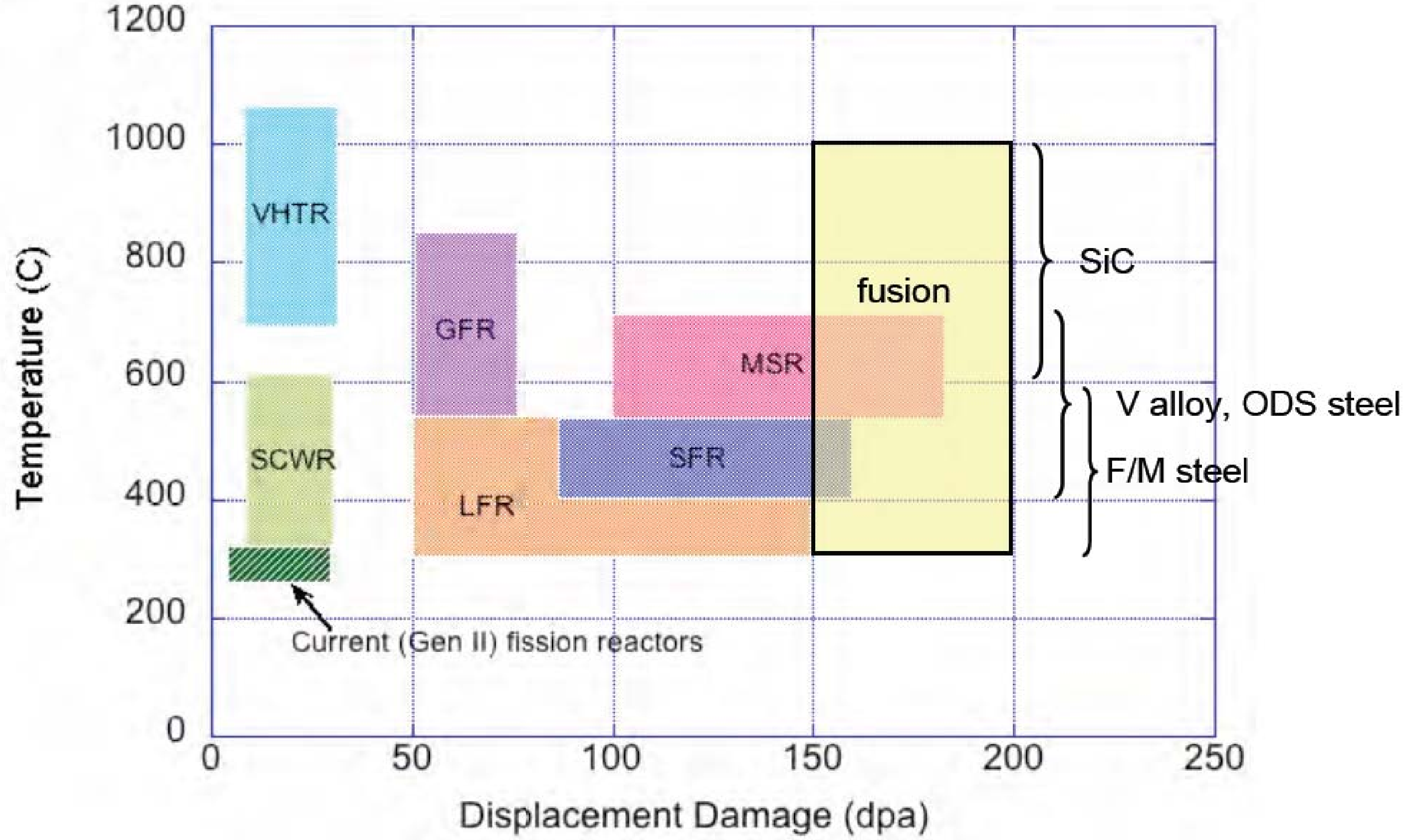
Main Aim:

1. Investigation of dislocation loop formation and growth in irradiated binary V-Fe alloys.
2. Physical Mechanisms of helium release during deformation of vanadium alloys doped by helium ions.

Content:

- Experimental data
- Physical Model
- Main Equations
- Results
- Comparison theoretical results with experimental data
- Summary

Comparison of Gen IV and Fusion Structural Materials Environments



Investigation of dislocation loop formation and growth in irradiated binary V-Fe alloys.

Background

- Vanadium-based alloys are considered as one of candidate structure materials for fusion reactors
- Understanding of physical mechanisms of an effect of solute atoms in these alloys on microstructure change is very important for the development of fusion material technology.

Objective

- Determine the effect of undersized impurity atoms on microstructure change and dislocation loop nucleation and growth in irradiated V-Fe alloys
- Investigation of the dose and temperature dependencies for evolution of dislocation microstructure change in irradiated V-Fe alloys

Experimental Procedure

Materials:

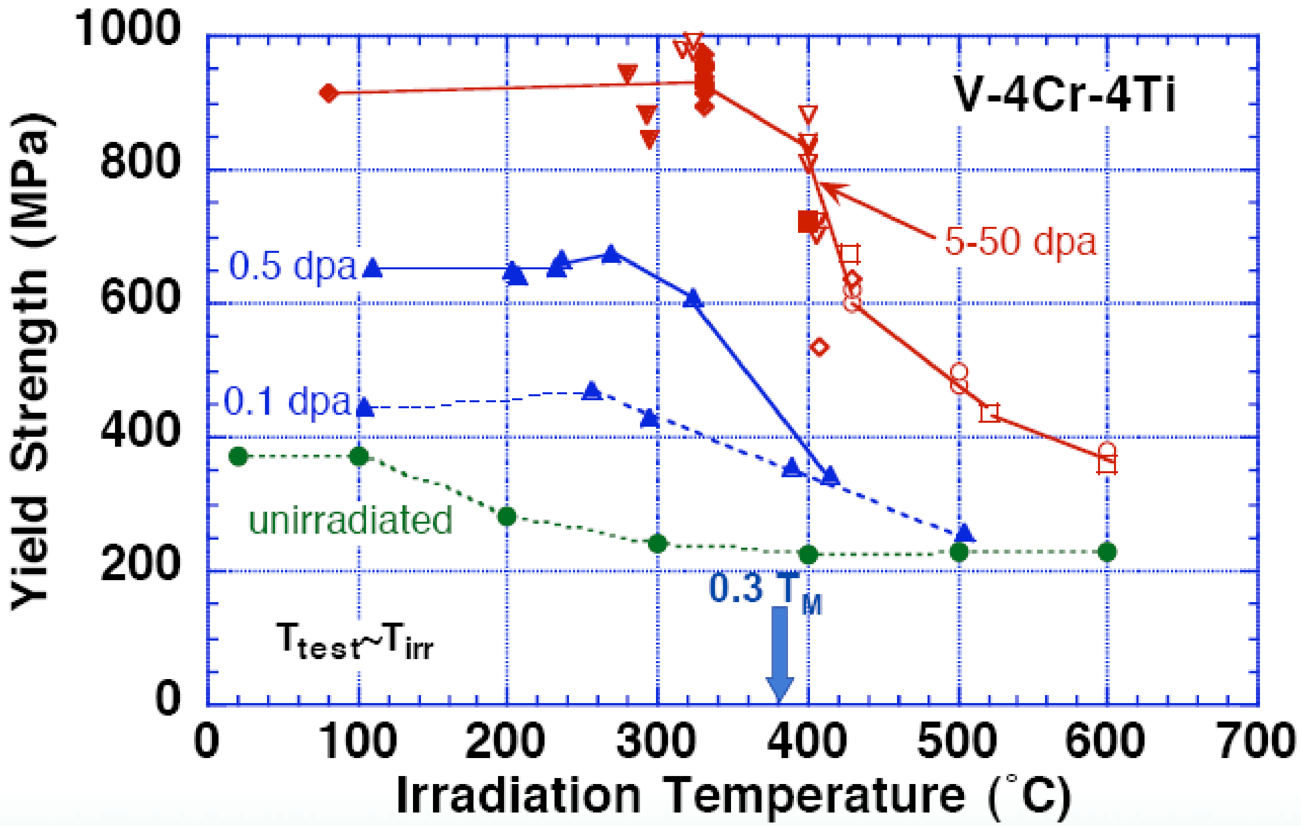
- Pure V (purity 99.9%),
- V-xFe (x=0.1, 0.2 0.3, 5 at%)
- V-yCr (y=0.1, 1.5 at%)

Irradiation Facility: ***JEM ARM 1250 of HVEM in Tohoku University, Japan***
Electrons: ***Energy up to 1.25 MeV***
Temperature: ***from RT to T = 493 K,***
Flux of electrons: ***4.3 x1022 to 3.6 x1023 e m-2 s-1***
Dose: ***Up to 3.36x1026 m-2***

Microstructure observations:

JEM ARM 1250 of HVEM
in Tohoku University, Japan

Radiation hardening in V-4Cr-4Ti



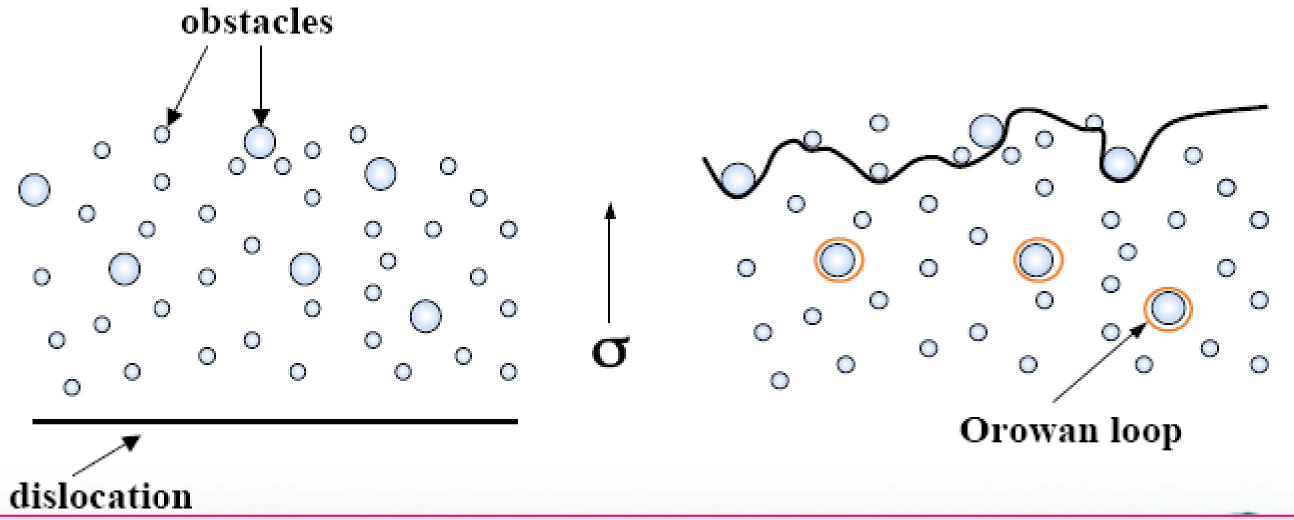
Effect of Dose and Irradiation Temperature on the Yield Strength of V-(4-5%)Cr-(4-5%)Ti Alloys

S.Zinkle (2004)

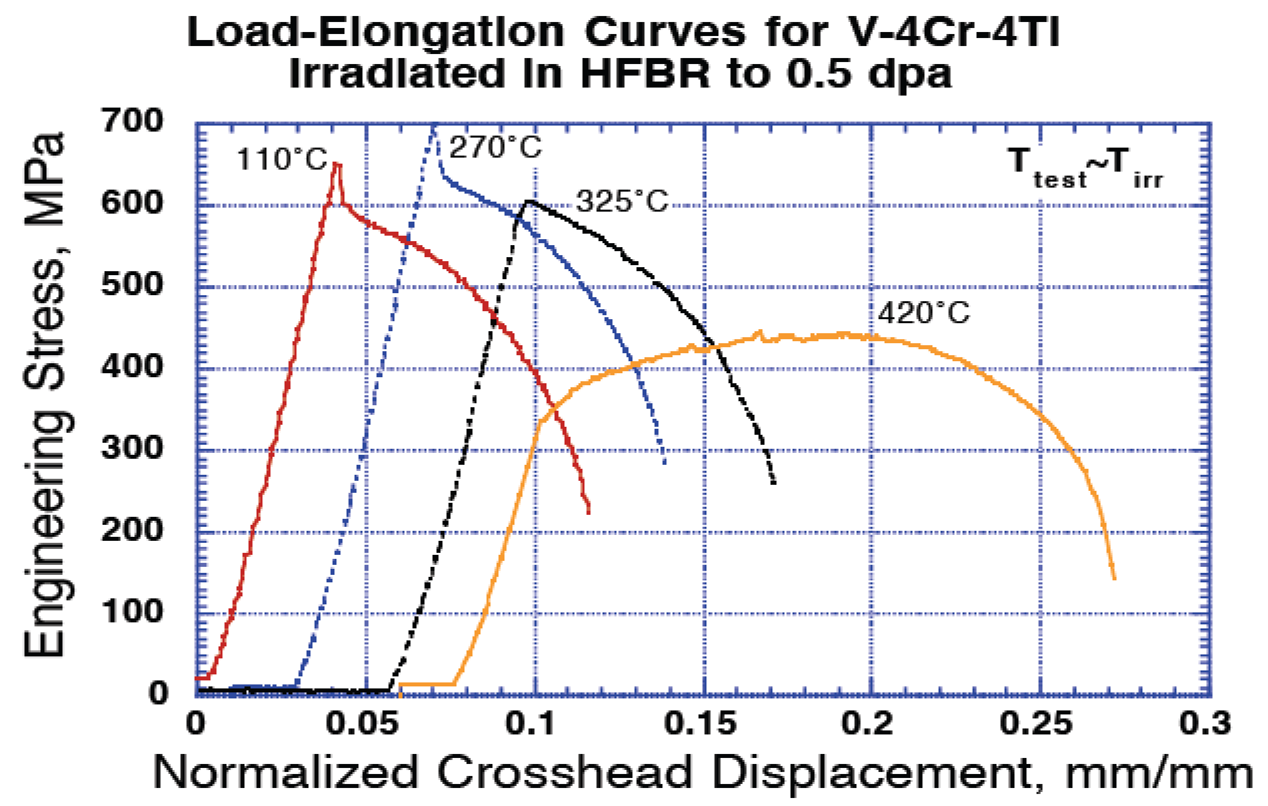
Radiation damage creates obstacles to dislocation motion

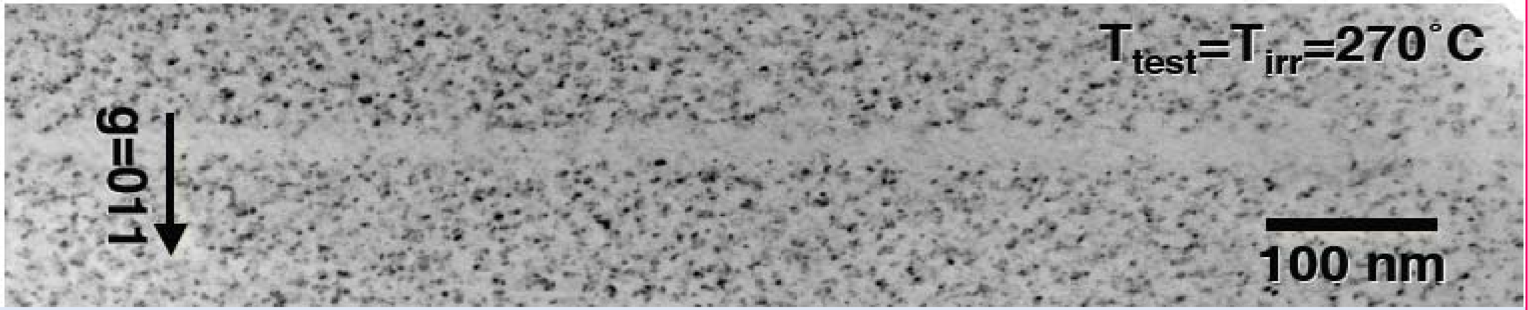
- point defects (≡ solute strengthening in alloys)
- small clusters and precipitates (≡ precipitates in alloys)
- impenetrable clusters (≡ Orowan strengthening in alloys)

- all give $\Delta\sigma_y$ proportional to $(\text{dose})^{0.3\text{-}0.5}$

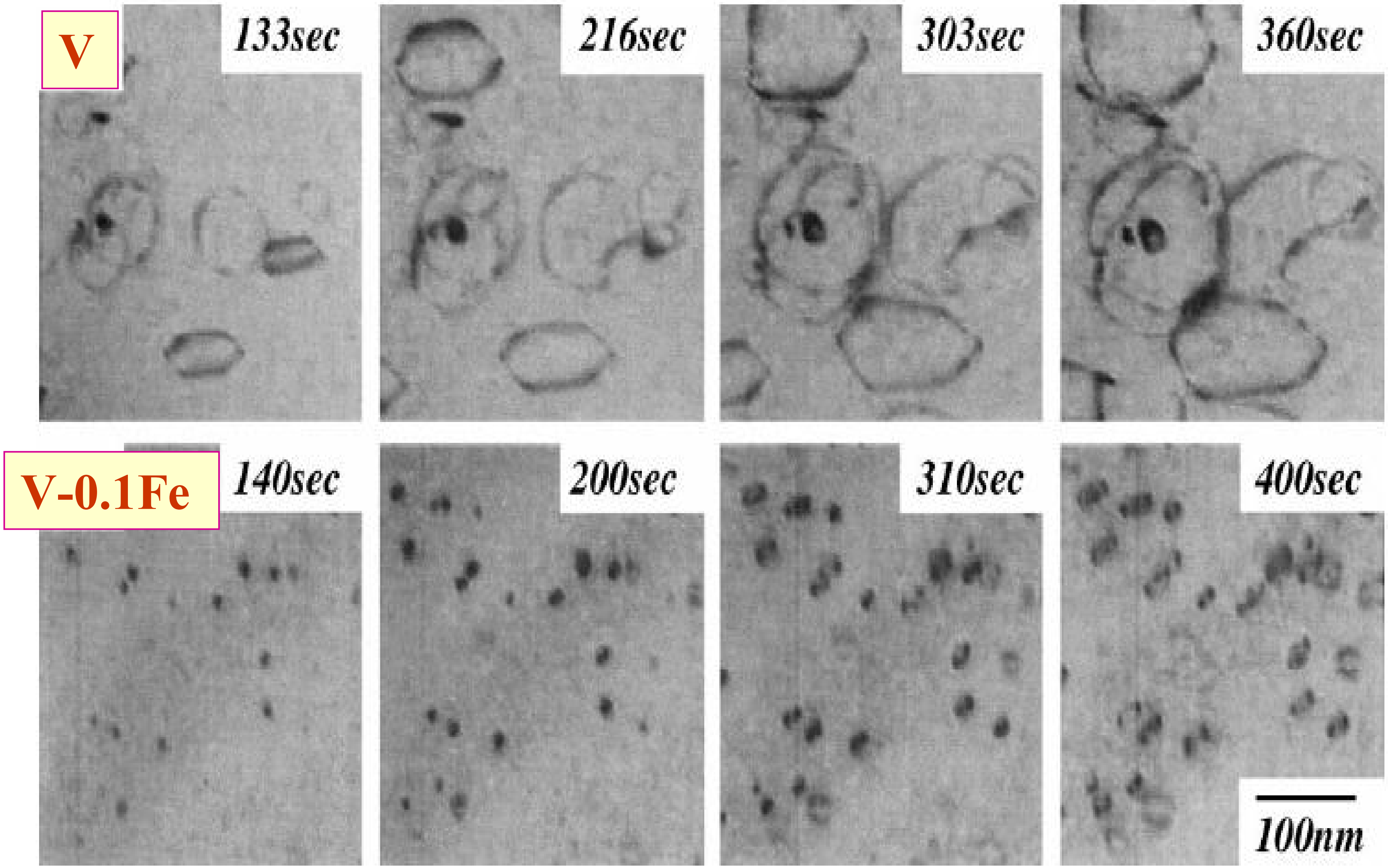


Irradiated Materials Suffer Plastic Instability (due to Dislocation Channeling?)

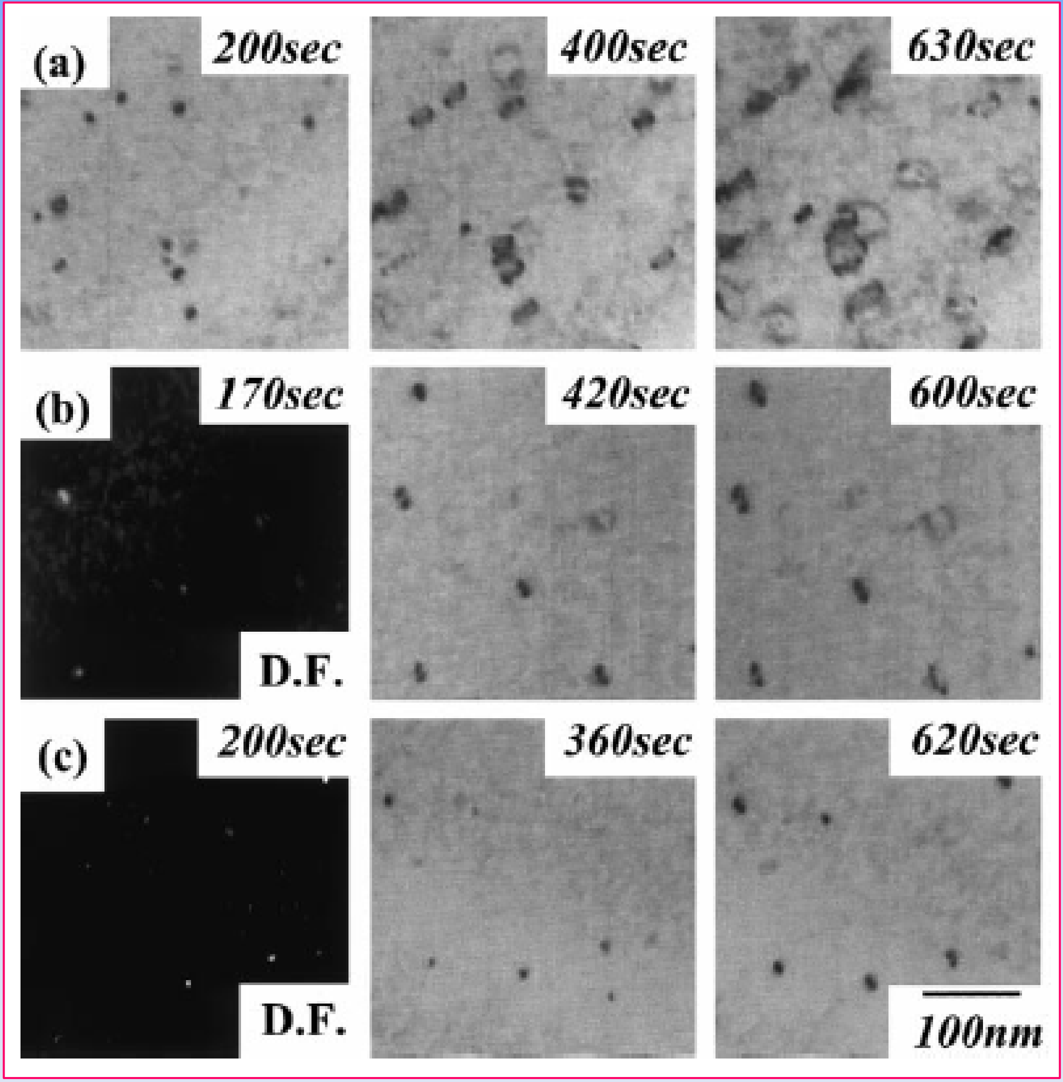




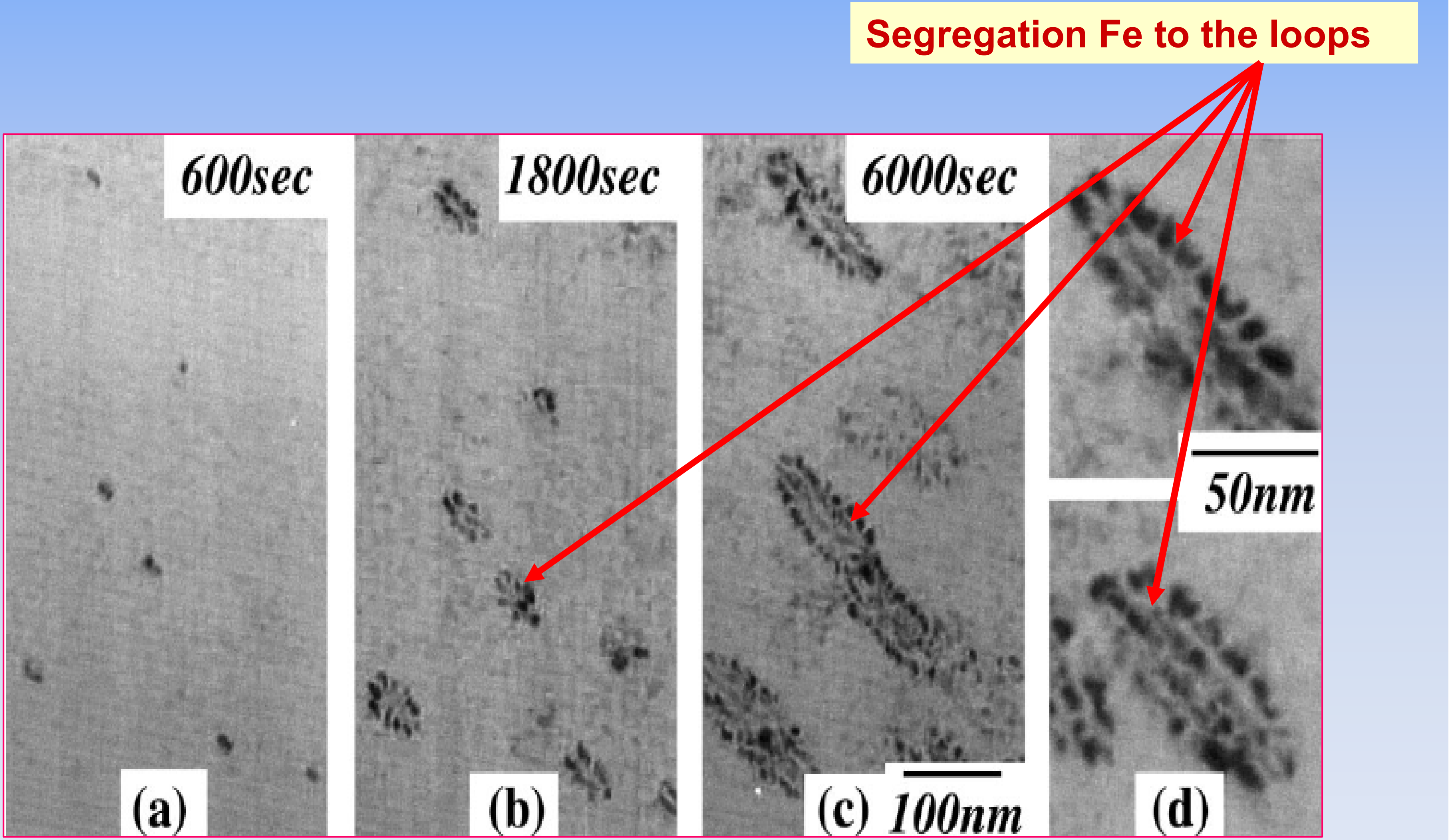
Microstructure evolution in pure V and V-0.1Fe during electron irradiation at T=493K and beam intensity of 2.1x1023 e / m2 s



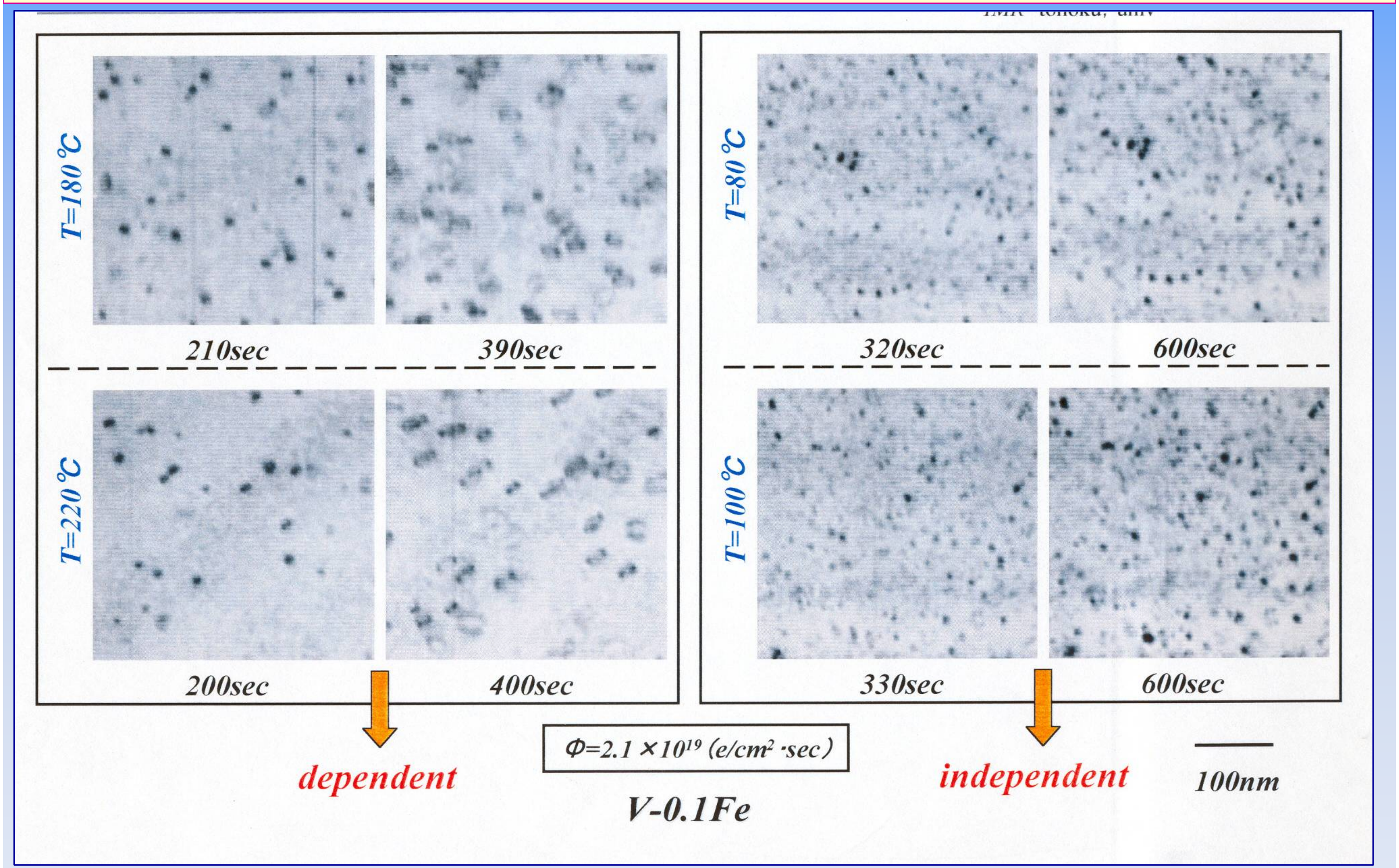
Typical microstructural evolution in V-0.1Fe (a), V-0.3Fe (b), V-5Fe (c) during electron irradiation at 493K.



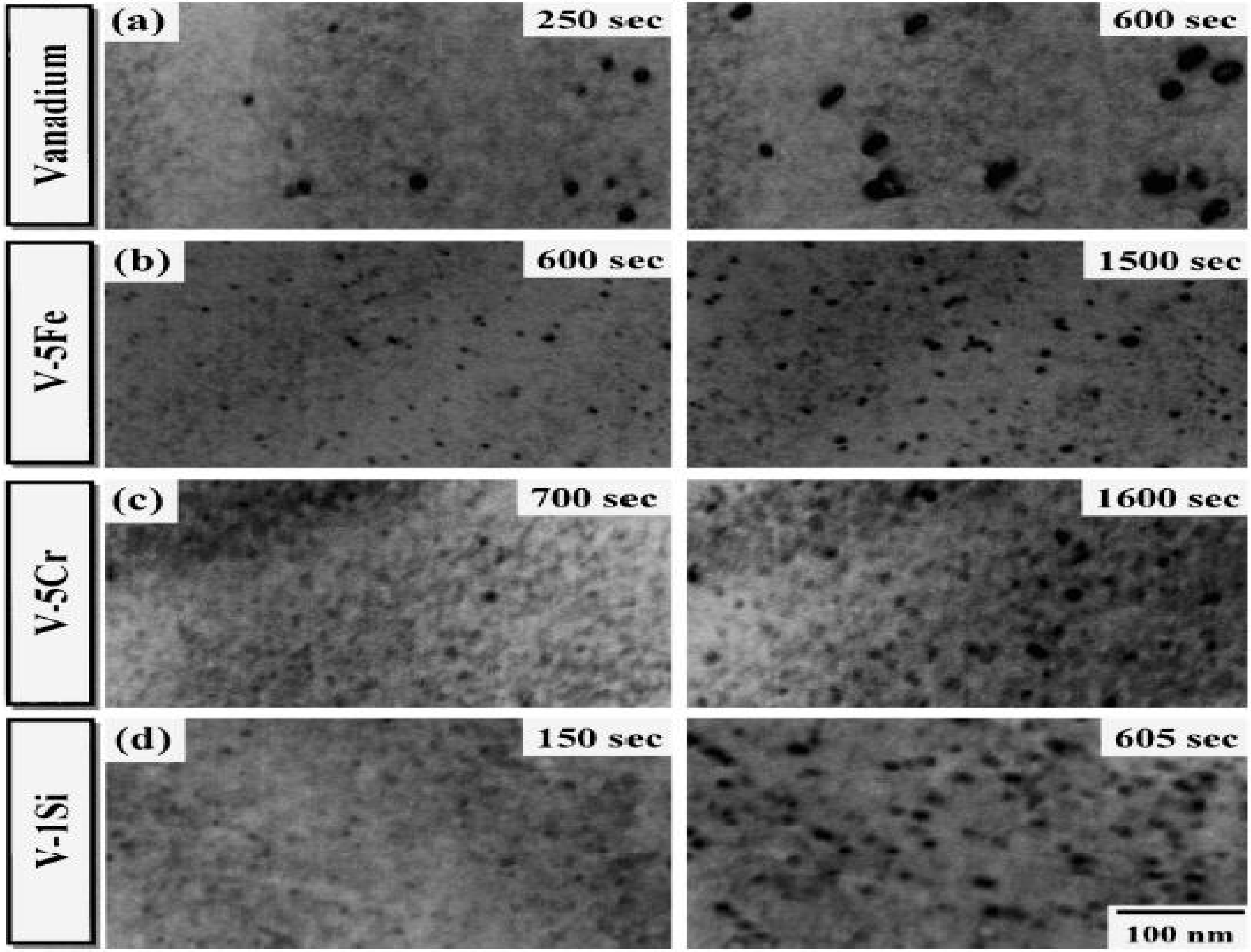
Dislocation loop evolution in V-5Fe during electron irradiation at different doses and at 523 K.



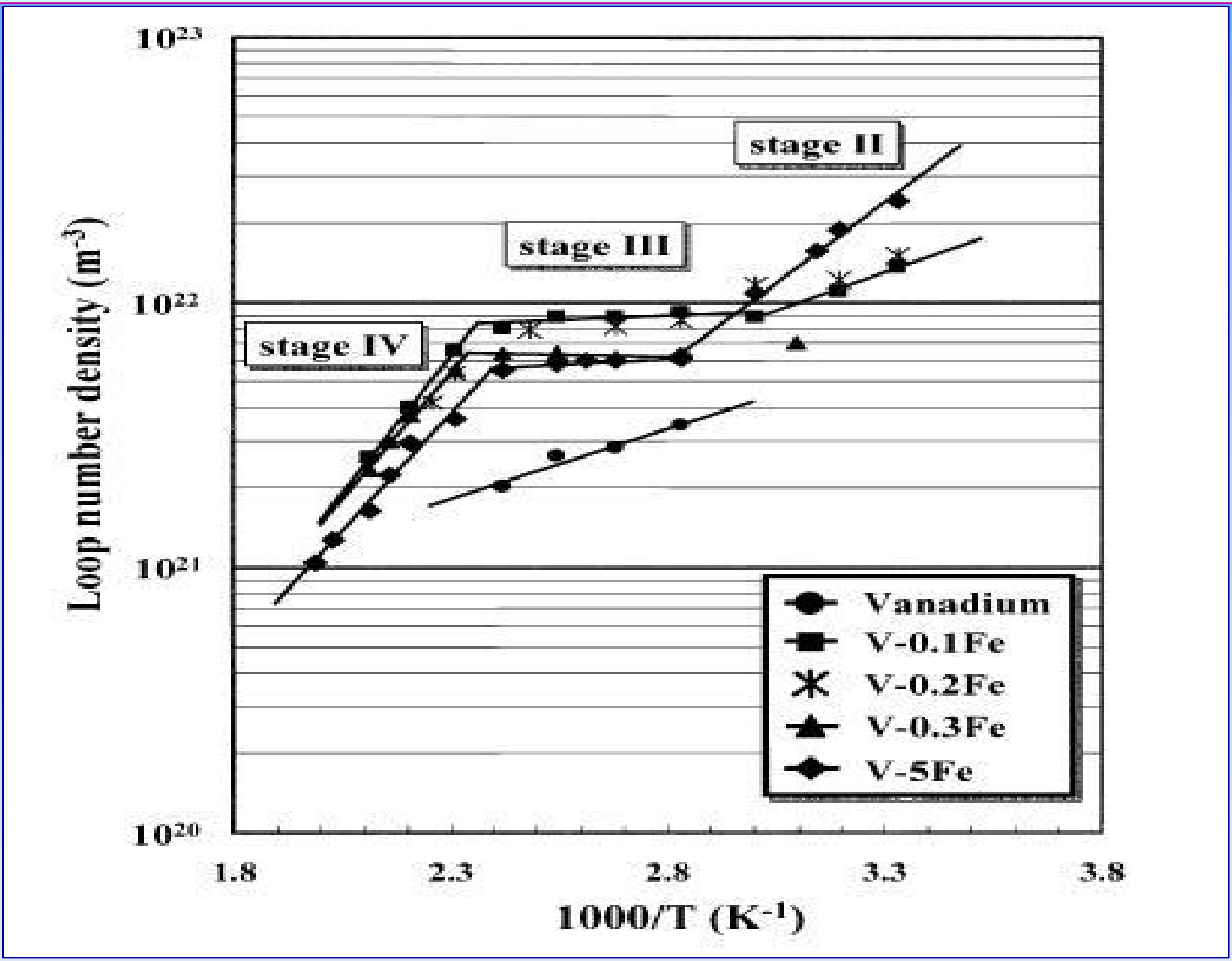
Dependence of loop number density in V-0.1Fe on irradiation temperature



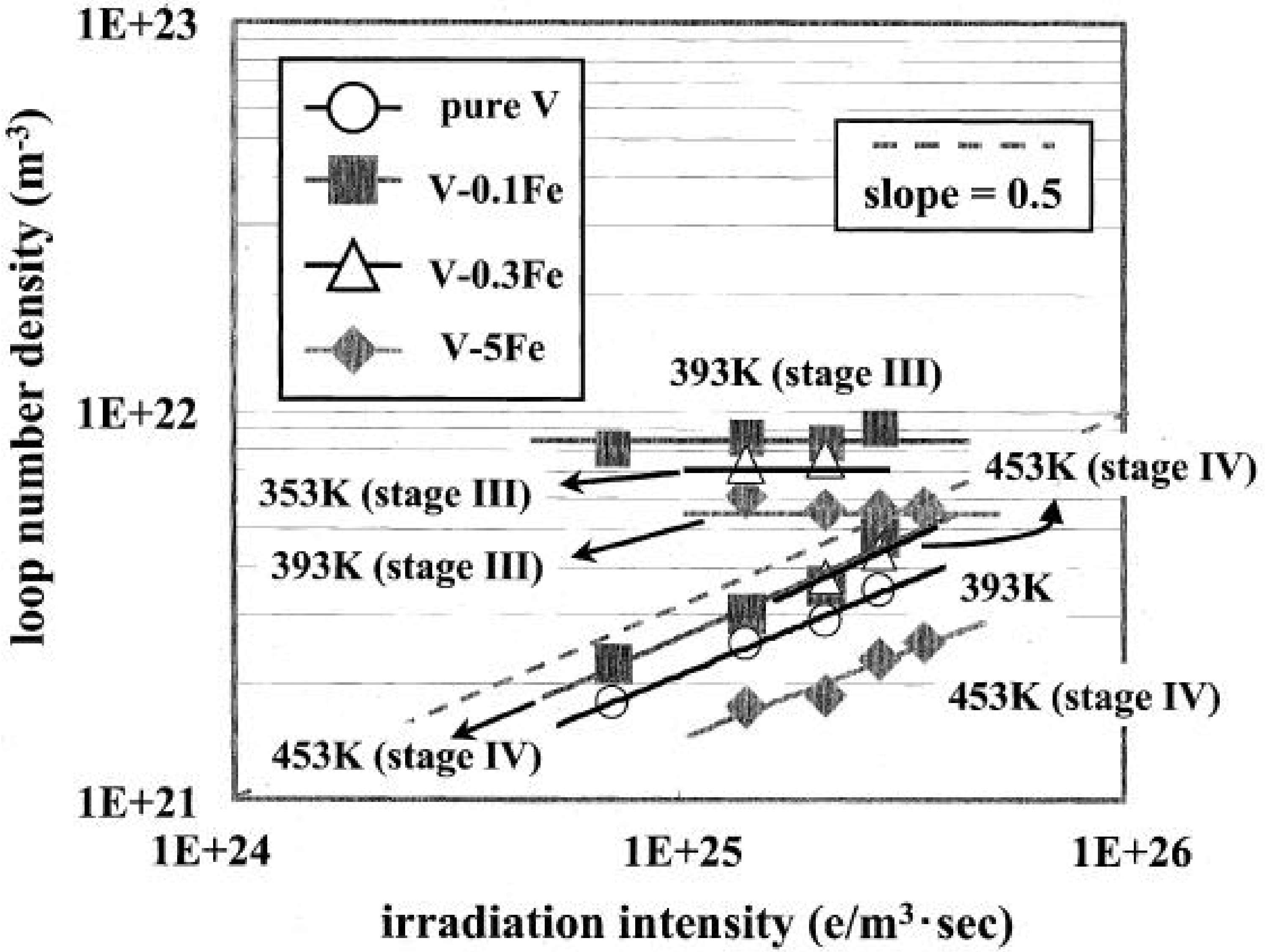
Microstructure change in V, V-5Fe, V-5Cr and V-1Si at electron fluxes: (a)-1.1x1023 em-2s-1, (b)-(d) 2.1x1023 em-2s-1 and T=393 K



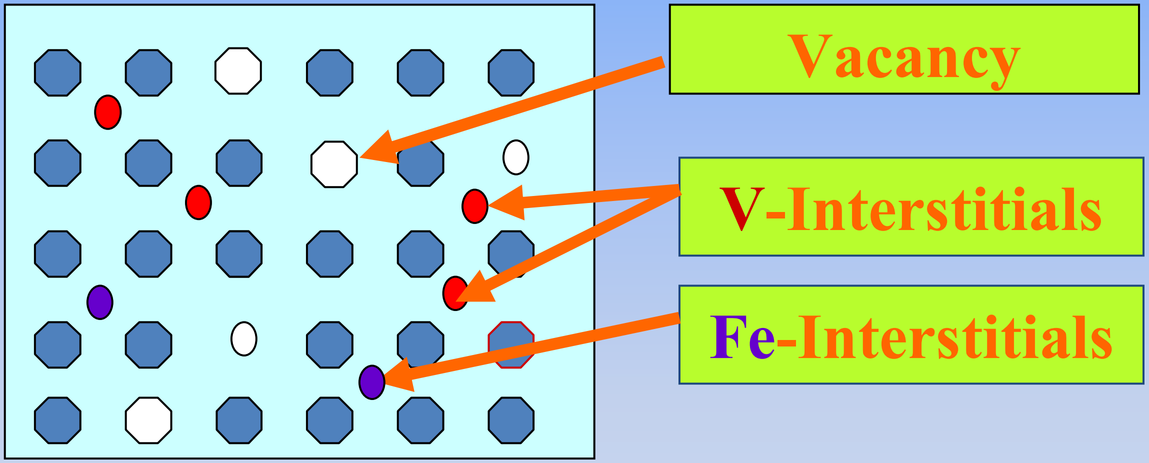
Arrenious plot of loop number density in V and V-Fe alloys irradiated at electron flux 2.1x1023 em-2s-1



Dependence of loop number density on irradiation intensity in V and V-Fe alloys at various temperatures



Physical Model

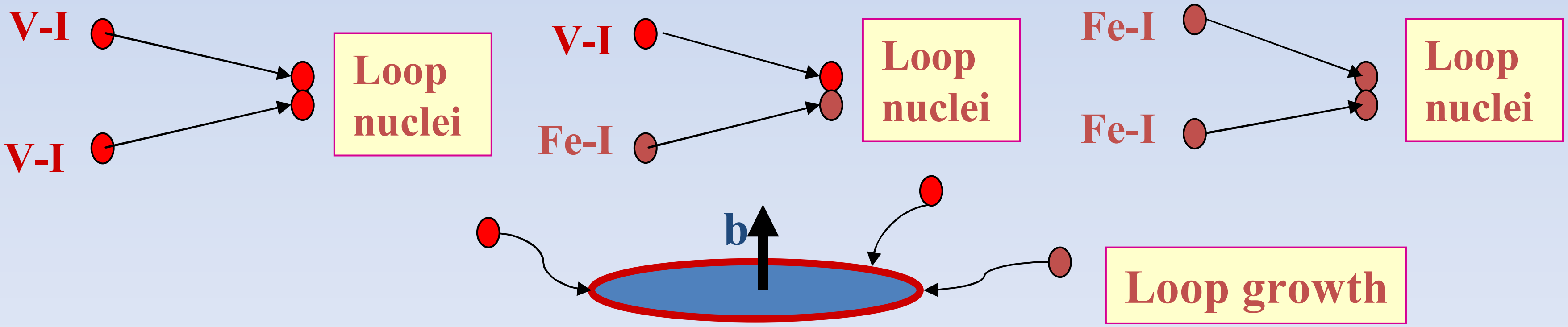


Vacancy

V-Interstitials

Fe-Interstitials

Mechanism of dislocation loop nucleation in V-alloys



V-I

V-I

Loop nuclei

V-I

Fe-I

Loop nuclei

Fe-I

Fe-I

Loop nuclei

b

Loop growth

The system of equations described the nucleation and growth of dislocation loops in irradiated V-alloys

$$\frac{dC_{i1}}{dt} = G_1 - Z_{iv} M_{i1} C_{i1} C_v - Z_{il}(\rho_d + 2\pi R N_l) M_{i1} C_{i1} a^2;$$

$$\frac{dC_{i2}}{dt} = G_2 - Z_{iv} M_{i2} C_{i2} C_v - Z_{il}(\rho_d + 2\pi R N_l) M_{i2} C_{i2} a^2;$$

$$\frac{dC_v}{dt} = (G_1 + G_2) - Z_{iv}(M_{i1} C_{i1} + M_{i2} C_{i2}) C_v - Z_{vl}(\rho_d + 2\pi R N_l) M_v C_v a^2;$$

$$\frac{dN_l}{dt} = Z_{i1} M_{i1} C_{i1}^2 + Z_{i2} M_{i2} C_{i2}^2 + Z_{i1}(M_{i1} + M_{i2}) C_{i1} C_{i2} - \gamma_{12} M_{i1} N_l;$$

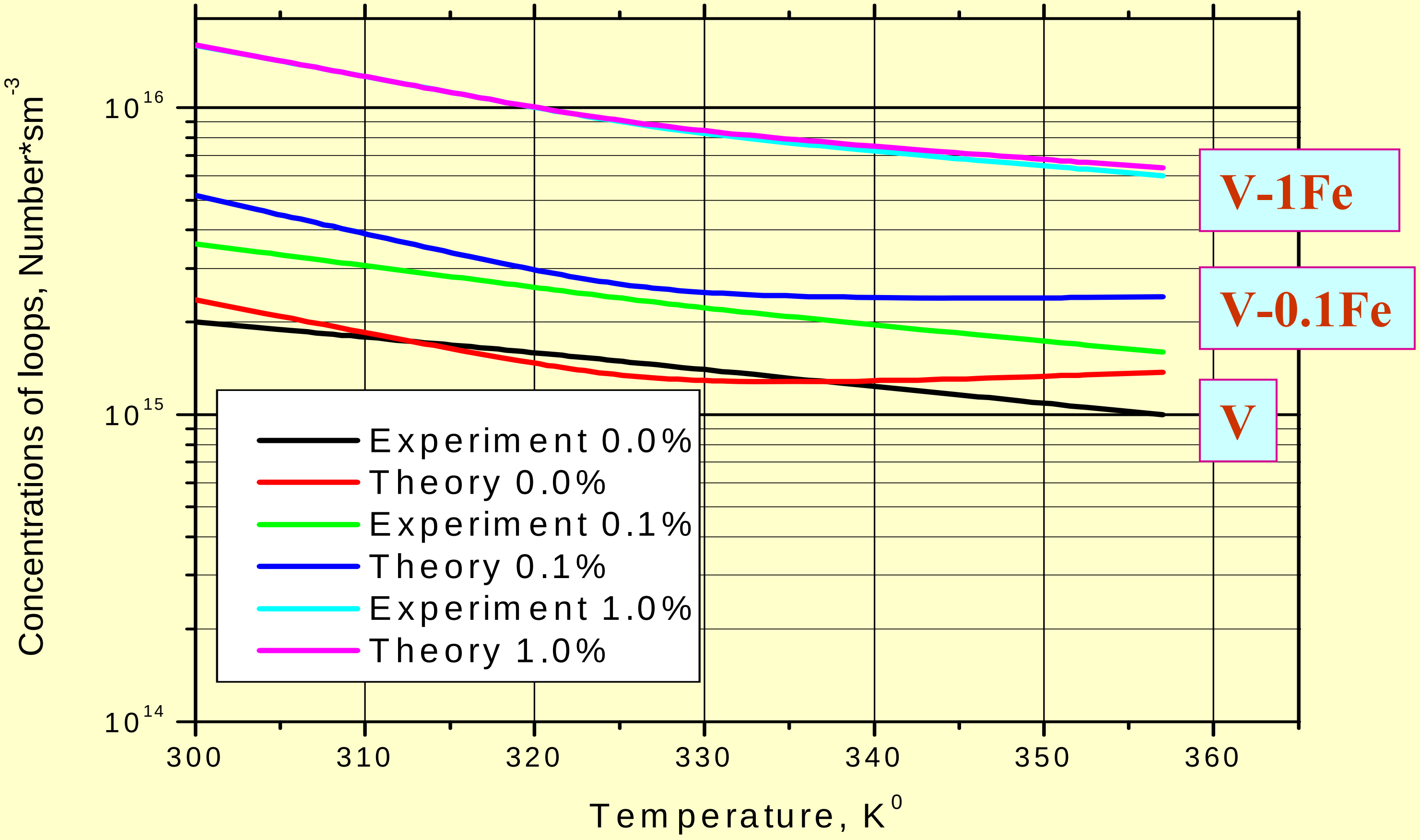
$$\frac{dR}{dt} = (Z_{il}(M_{i1} C_{i1} + M_{i2} C_{i2}) - Z_{vl} M_v C_v) a;$$

Ci1, Ci2 and Cv are the concentrations of self interstitials of V atoms, interstitials of Fe atoms and vacancies respectively,
G1 ,G2 are the generation rates of two types of point defects,
Mi ,Mv are the mobility of interstitials and vacancies,
a is the lattice spacing ρd is the dislocation density,
R,Nl are the radius and concentrations of dislocations loops,
Ziv, Zil, Zvl, Zii are the coefficients which characterize the interaction of point defects between itself and dislocations,

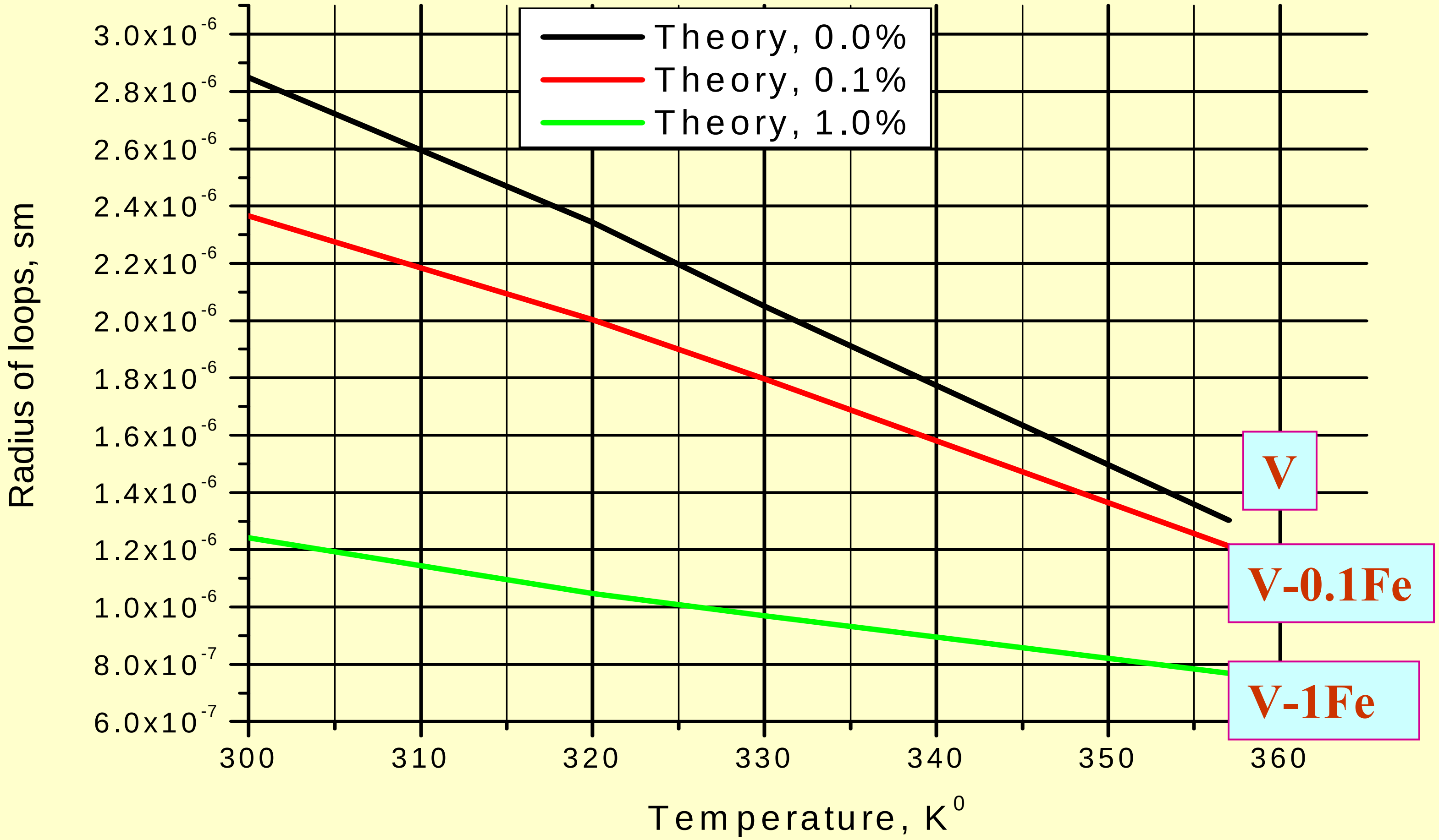
Main values used in numerical loop calculations of dislocation loop formation in irradiated V-Fe alloy

G1	3.31*10-4 V sec -1
G2	3.59*10-4 Fe sec -1
a	3.03*10-8 cm
p	3.13*10 9 cm-2
Emi1	0.37 eV
Emi2	0.57 eV
Emv	0.78 eV
Ziv	2.01
Z2i	3.08
Zil	6.25 (T=370K)
Zvl	2.82 (T=370K)

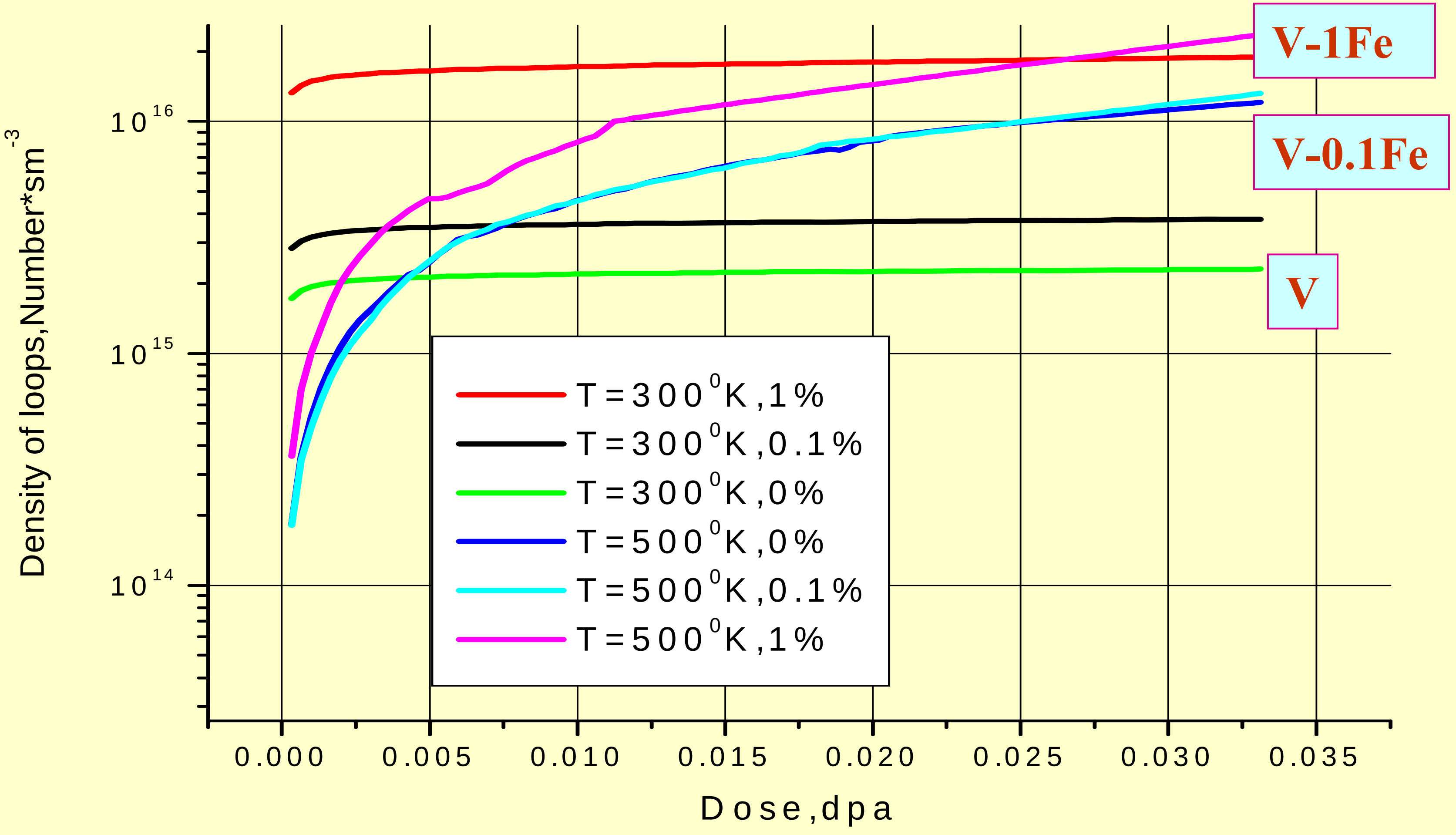
Comparison of experimental results and numerical calculations for temperature dependencies of dislocation loops densities in V-Fe alloys (Pure V, V-0.1Fe and V-1Fe)



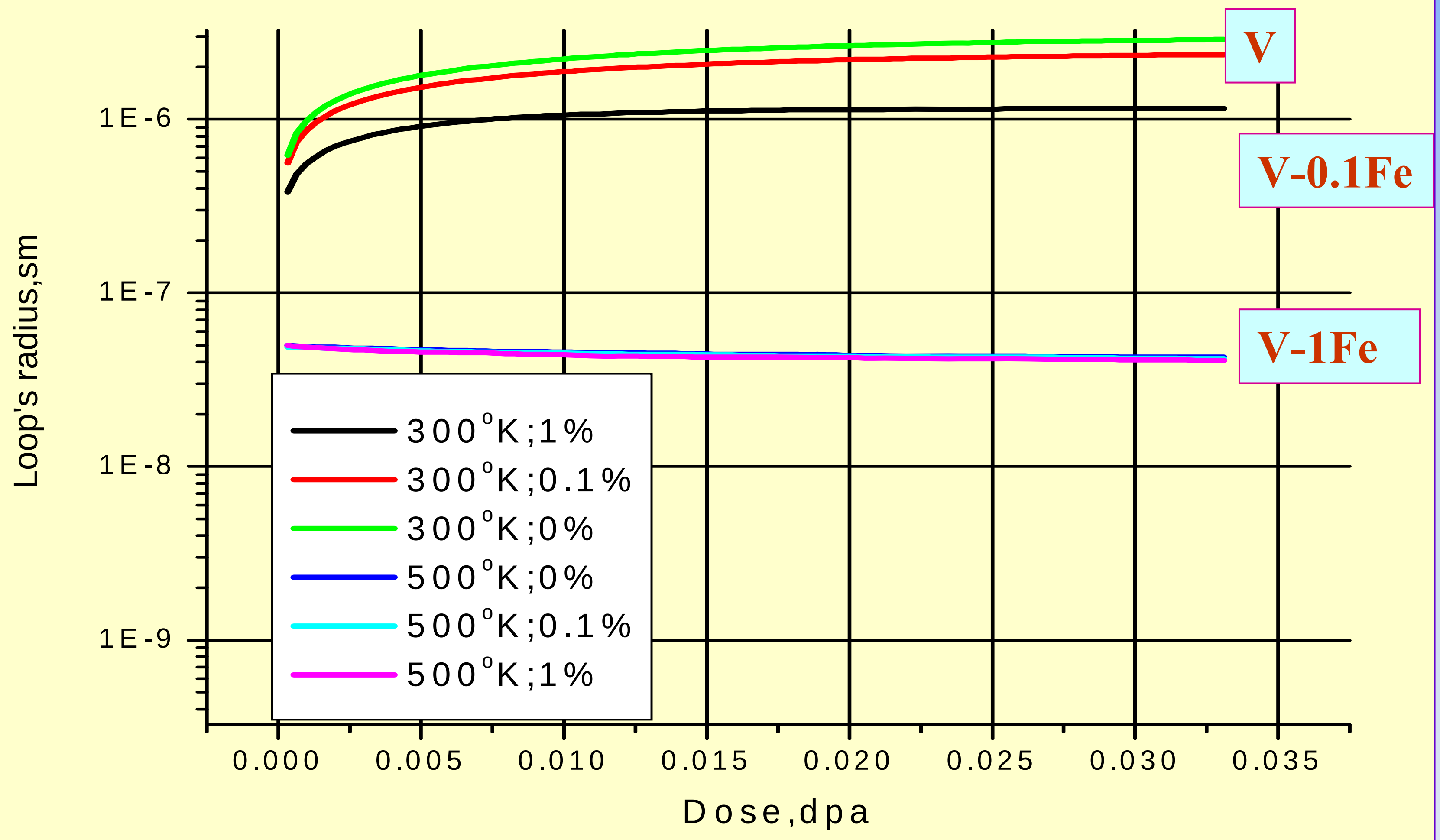
Results of numerical calculations for temperature dependencies of mean dislocation loop radius in V-yFe alloys (Pure V, V-0.1Fe and V-1Fe)



Results of numerical calculations for dose dependencies of dislocation loops densities in V-x Fe alloys (Pure V, V-0.1Fe and V-1Fe)at temperatures: T=300 K and T=500 K



Results of numerical calculations for dose dependencies of mean dislocation loop radius in V-x Fe alloys (Pure V, V-0.1Fe and V-1Fe)



Summary

☆ The microstructure evolution and dislocation loop formation and growth during electron irradiation have been studied by using HVEM and numerical modeling in pure V and V-Fe alloys in a wide range of Fe concentration in order to examine the interaction between V-SIAs and Fe atoms.

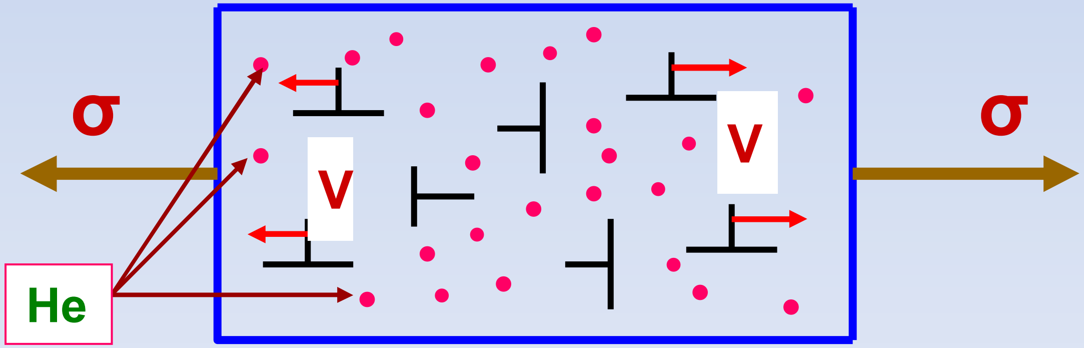
☆ Effect of Fe-solutes (undersized atoms) in binary V-Fe alloys on loop nucleation is very significant and dominates the loop nucleation, indicating that Fe-atoms trap V-SIAs and leading to the appearance of the strong temperature dependence.

☆ The theoretical modeling in pure V and V-Fe alloys based on the di-atomic nucleation model of dislocation loops with the migration energies of self interstitial V atoms: *Emi1* = 0.37 eV and Fe atoms: *Emi2* = 0.57 eV give the same temperature dependence for dislocation loop density as experimental data.

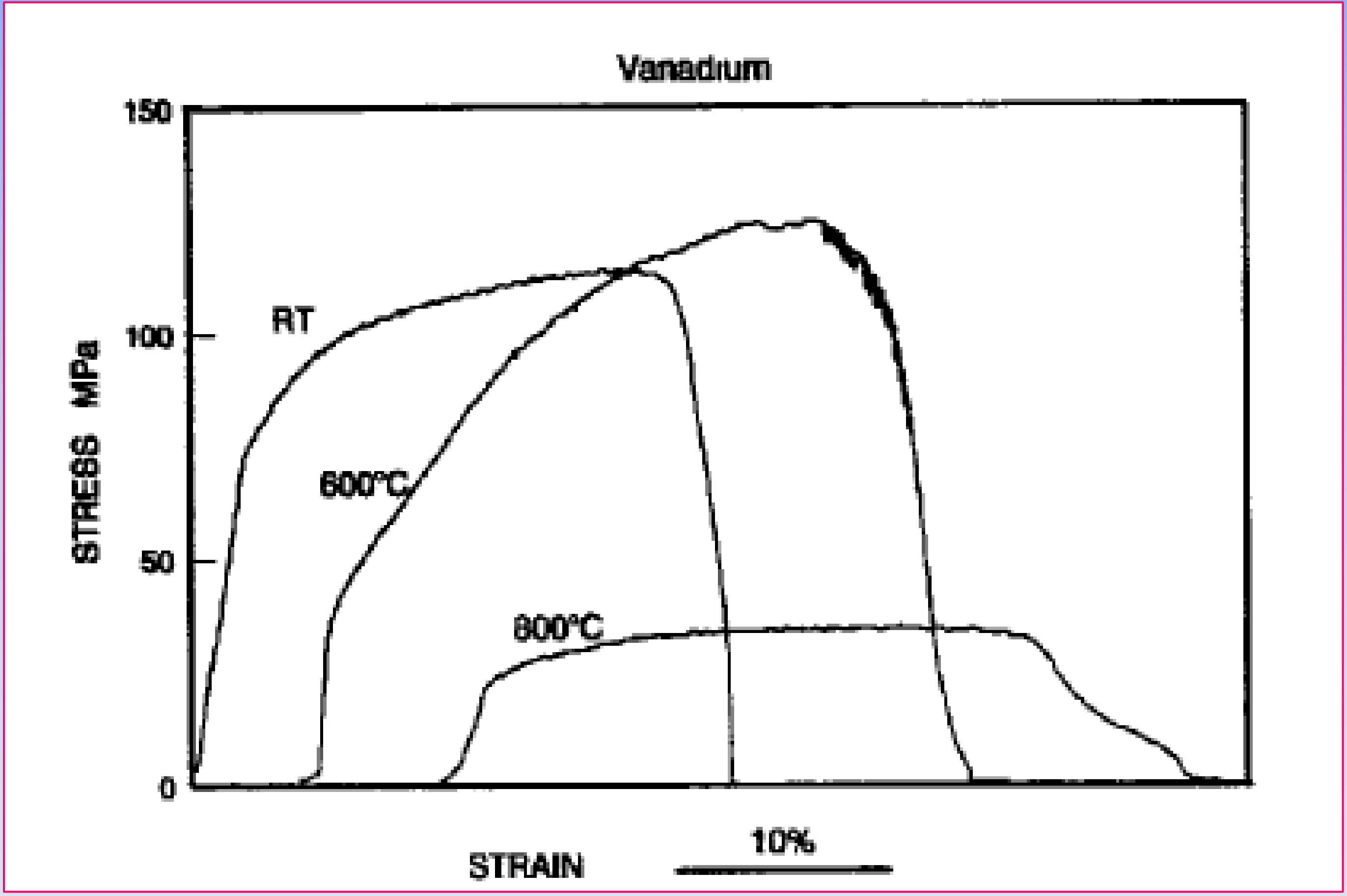
2.Physical Mechanisms of helium release during deformation of vanadium alloys doped by helium ions.

Experimental results (H.Matsui, 1989-1991):

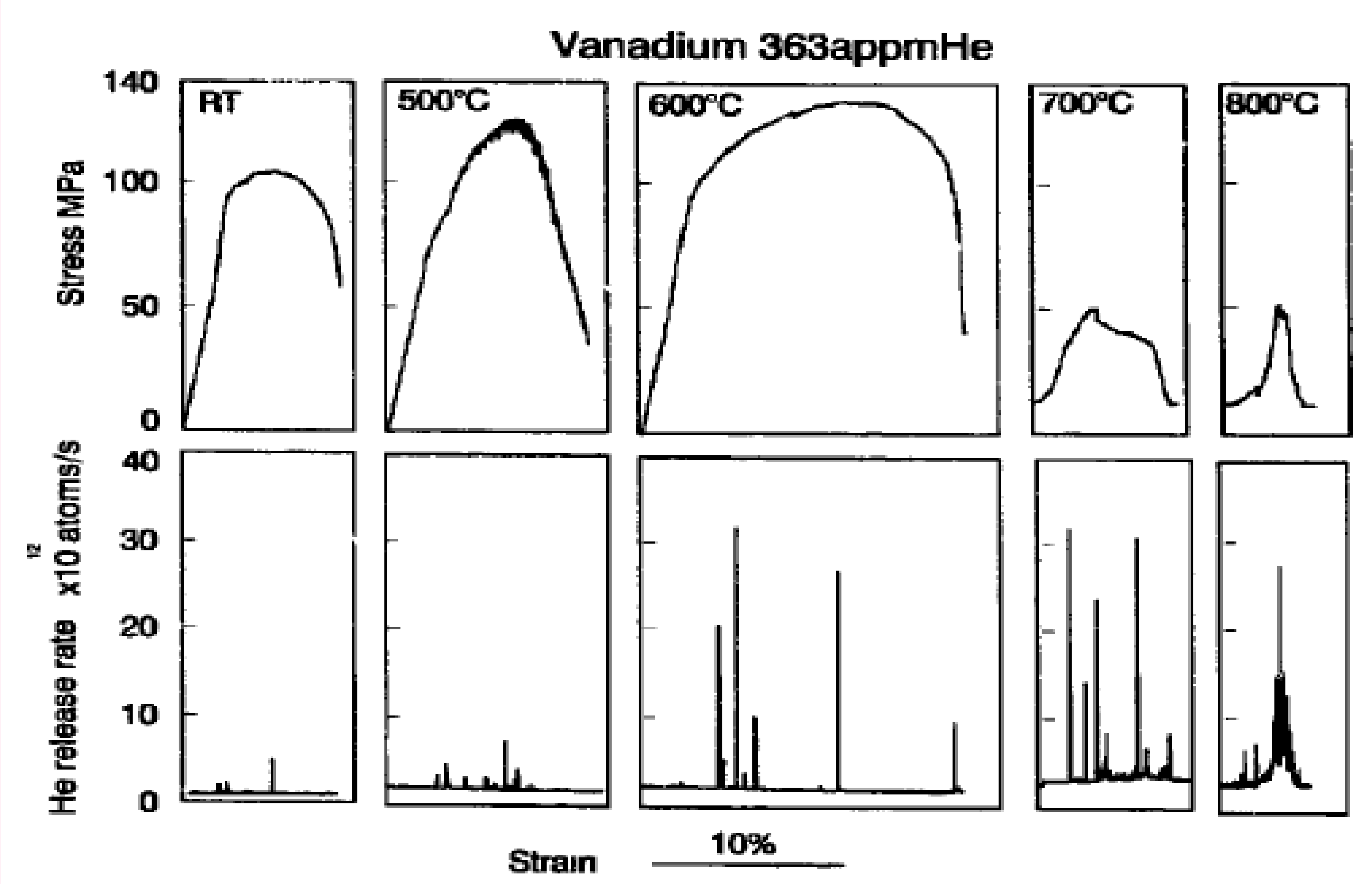
- Mechanical tests – **dε/dt =** $10^{-3} - 10^{5} s^{-1}$
- Helium implantation by the tritium trick method
- Helium releasing during plastic deformation
- Strong temperature dependence
- Helium release depends on alloy composition



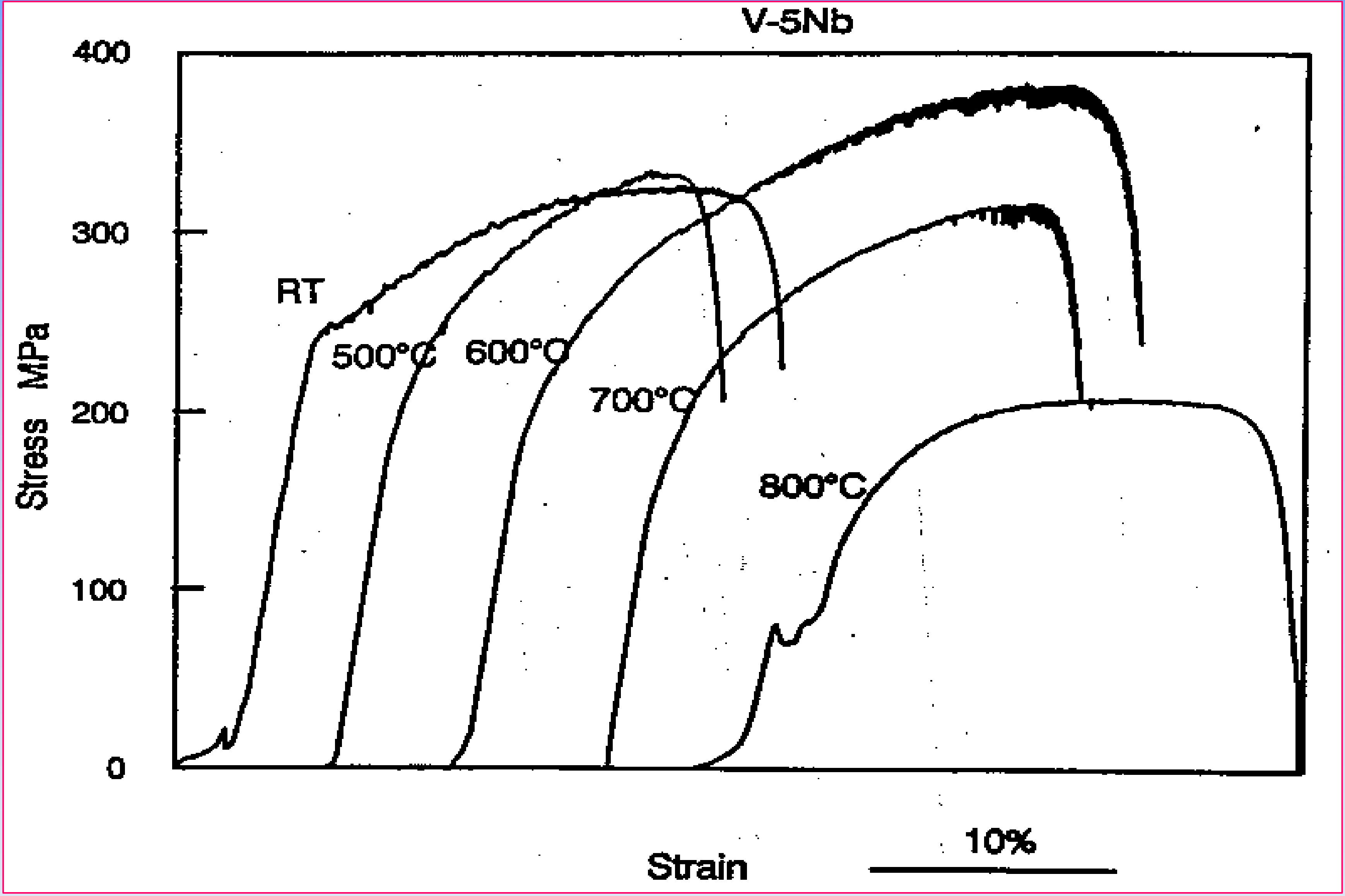
Stress-strain curve of helium free vanadium



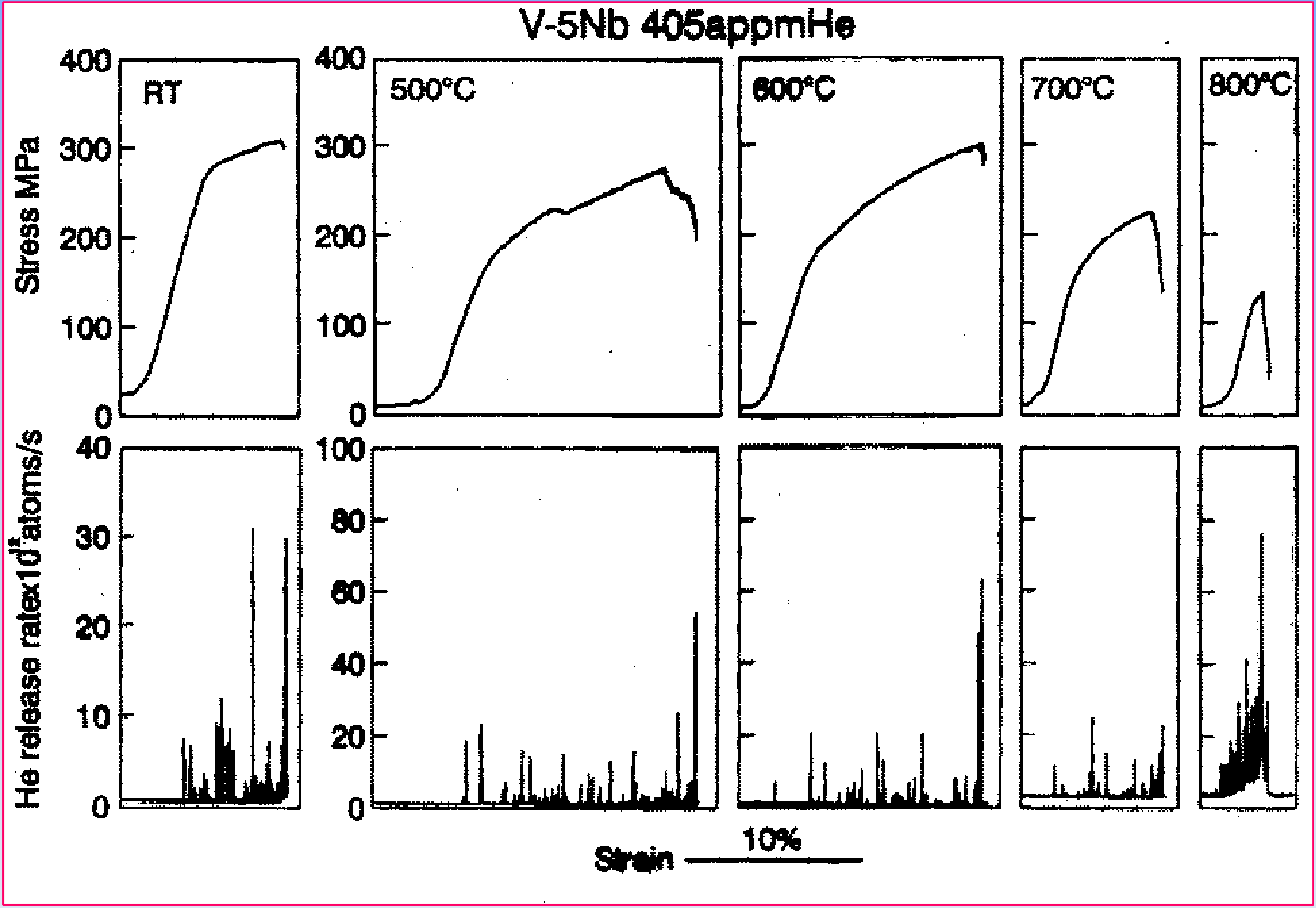
Stress-strain curves (top) and helium release (bottom) curves of helium doped vanadium



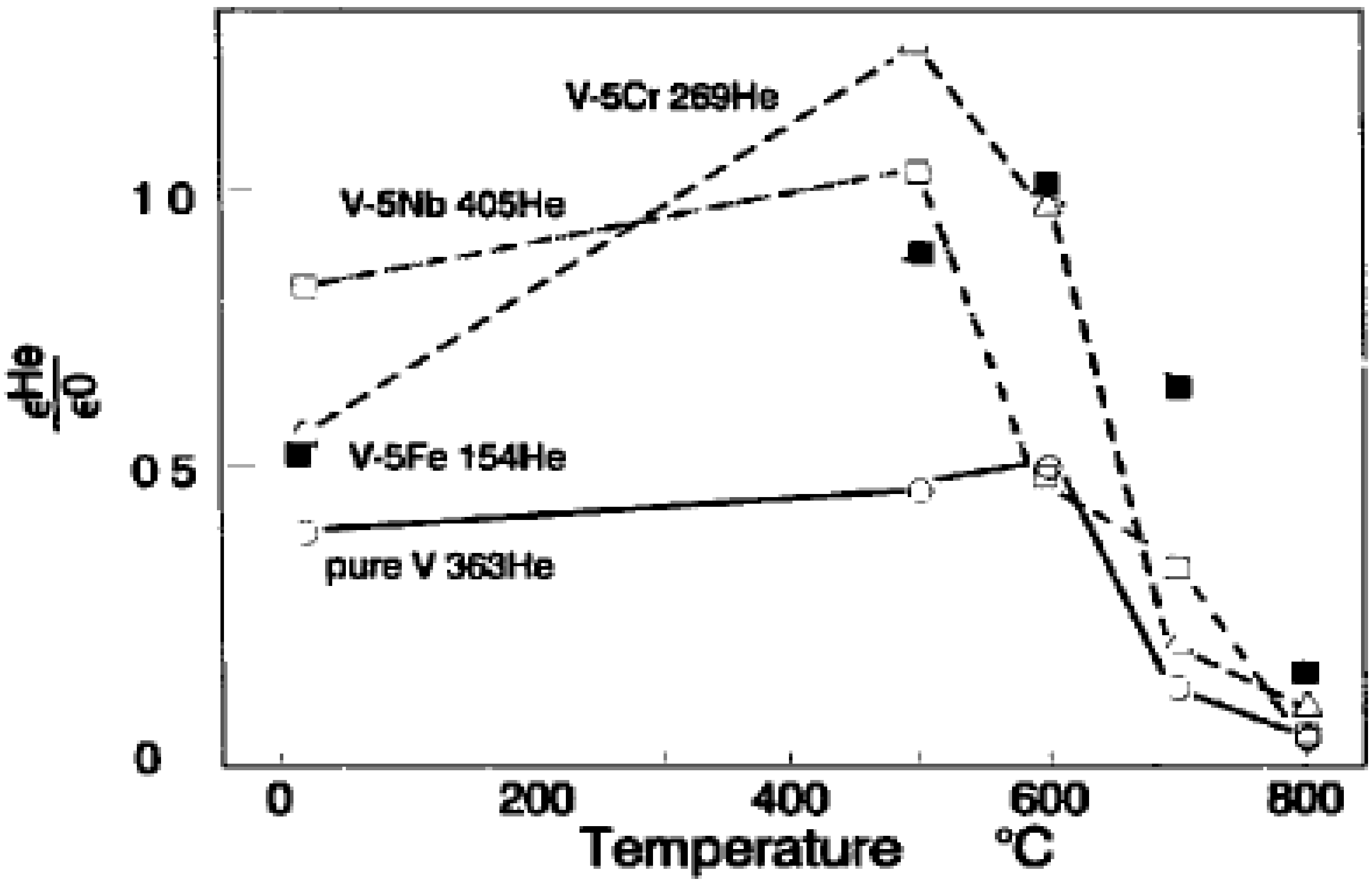
Stress-strain curve of helium free V-5Nb



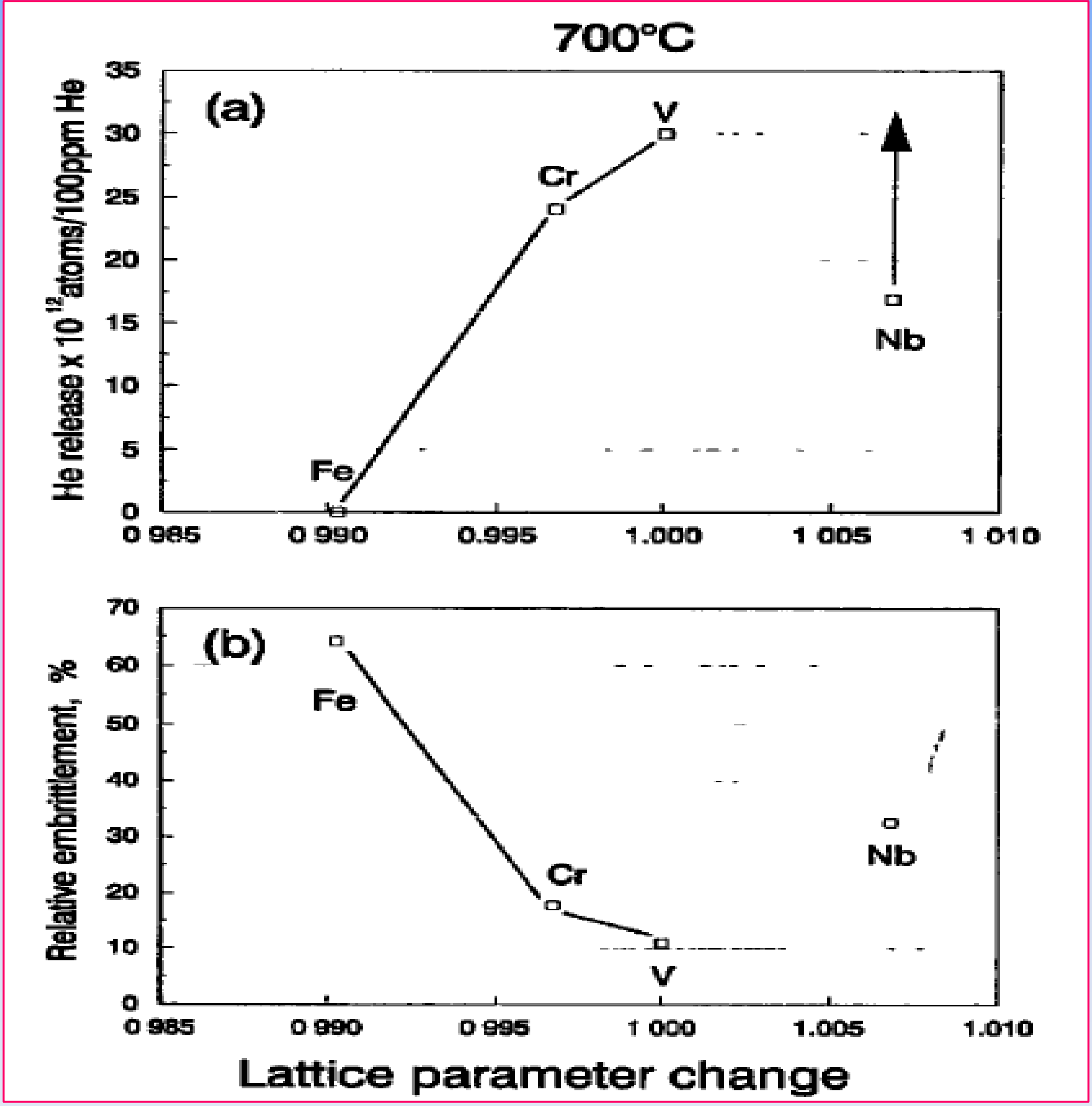
Stress-strain curves (top) and helium release (bottom) curves of helium doped V-5Nb



Helium embrittlement (represented by elongation of helium doped specimen divided by that of the helium-free specimen) of V-alloys as a function of temperature

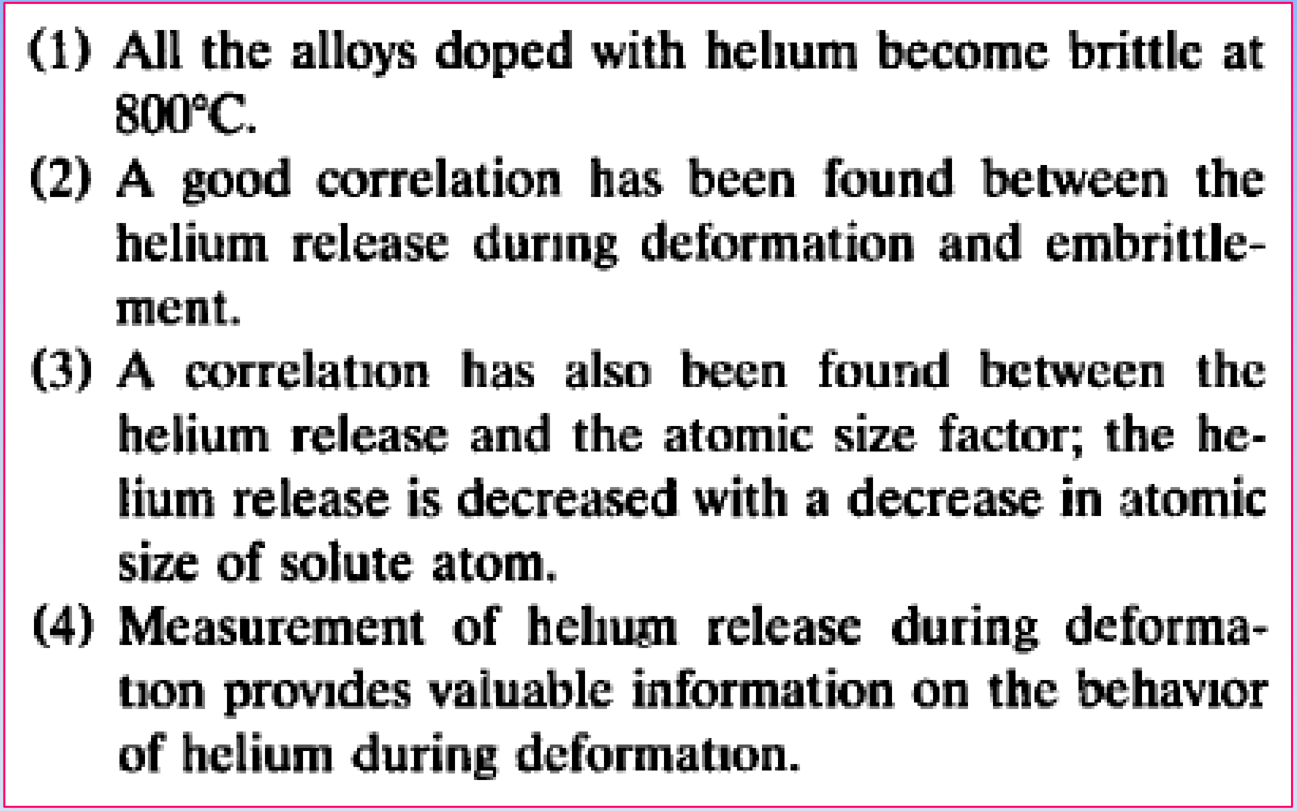


Correlation of helium release during deformation (a) and relative ductility (b) with the lattice constant normalized to pure vanadium



	a_R	a_L
V	1.71 A	3.03 A
Cr	1.66 A	2.88 A
Fe	1.56 A	2.86 A

Conclusion from experimental tests



(1) All the alloys doped with helium become brittle at 800°C.

(2) A good correlation has been found between the helium release during deformation and embrittlement.

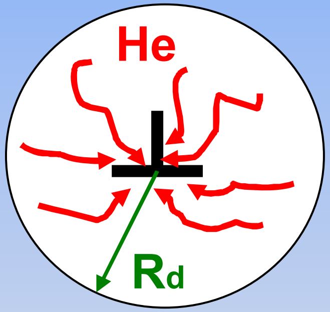
(3) A correlation has also been found between the helium release and the atomic size factor; the helium release is decreased with a decrease in atomic size of solute atom.

(4) Measurement of helium release during deformation provides valuable information on the behavior of helium during deformation.

Helium release due to dislocation-dynamic mechanisms

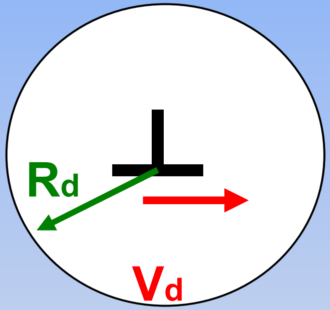
1. Characteristic times of processes:

(A.Ryazanov, H.Matsui,1999)



$$\tau_{He} \approx \frac{R_d^2}{D_{He}}$$

$$R_d = (\pi \rho_d)^{-1/2}$$



$$\tau_d \approx \frac{R_d}{V_d}$$

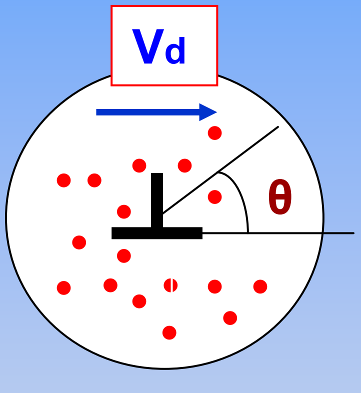
τ_{He} - characteristic time of He accumulation on dislocation
D_{He} - diffusion coefficient of He
τ_d - characteristic time of dislocation motion
ρ_d - dislocation density
V_d - dislocation velocity

$$\frac{d\varepsilon}{dt} = b\rho_d V_d$$

1) "Fast" helium: $\tau_{He} \le\le \tau_d$

2) "Slow" helium: $\tau_{He} \ge\ge \tau_d$

2) “Fast” helium (tritium trick method). Helium atoms in interstitial positions: $\tau_{He} \leq\leq \tau_d$



Main Equations:

$$\frac{\partial C}{\partial t} + div\,\vec{j} = 0$$

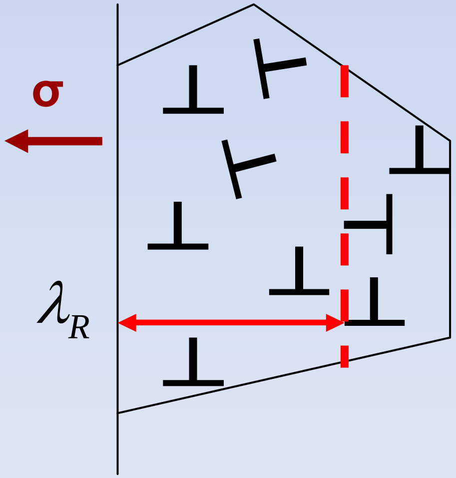
$$\vec{j} = -D\nabla C - \frac{DC}{kT}\nabla U - \vec{V}_d C$$

$$U = \frac{A}{kT}\frac{\sin\theta}{r},\ A = \frac{4}{3}\mu\varepsilon r_0^3 b\frac{1+\nu}{1-\nu}$$

$\vec{j}$ is the current of helium, T is the temperature,

***U* is the interaction energy of He with dislocation**

Boundary conditions: $C(R_d) = C_0, C(r_0) = C_{th} = 0$



$$\lambda_R = V_d \tau_R$$

τ_R is the rapture time

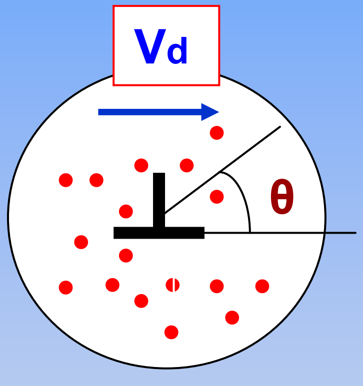
$$\tau_R \approx \frac{\varepsilon_R}{d\varepsilon / dt}$$

$$N_{tot} \approx \frac{\pi C_0 S_0 R_d}{2\ \ln(R_0/2R_d)}$$

$$N_{tot} \propto \frac{1}{\ln(\frac{A}{T})}$$

C₀ = 300 appm, T = 800 K, $N_S \approx 2.10^{13}, N_{tot} \approx 2.10^{15}$

3) “Slow” helium (saturation of He on cyclotron)
Helium atoms in substitution positions: $\tau_{He} \geq\geq \tau_d$



Main Equations:

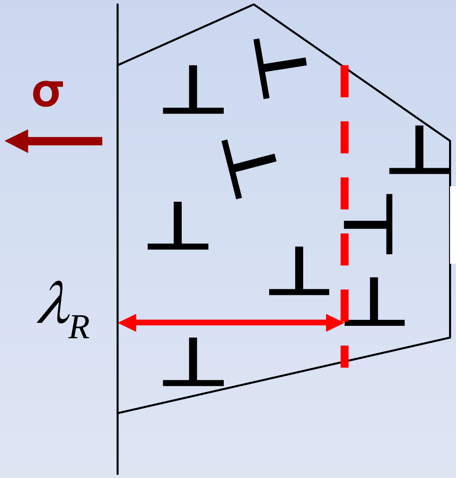
$$\frac{\partial C}{\partial t} + div\,\vec{j} = 0$$

$$\vec{j} = -D\nabla C - \vec{V}_d\,C$$

$$D\Delta C + (\vec{V}_d, \vec{n})C = 0$$

$\vec{j}$ is the current of helium, T is the temperature,

Boundary conditions: $C(R_d) = C_0, C(r_0) = C_{th} = 0$



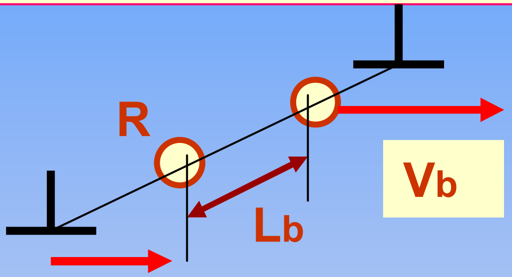
$$N_{tot} \approx 2S_0\varepsilon_p C_0 L\left\{\pi\frac{D\rho_d}{\dot{\varepsilon}_0}\frac{r_0}{b}\right\}^{1/2},$$

$$N_{tot} \propto \exp\left(-\frac{E_m}{2T}\right)$$

C_0 = 300 appm, T = 800 K, L=10 µm, S_0 =0.15cm2, E_{ms} = 1.5eV

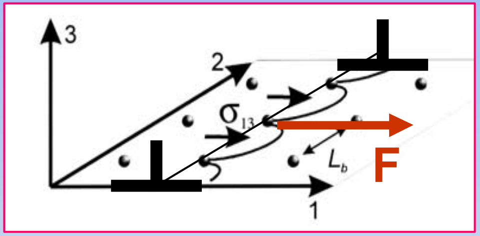
$$N_S \approx 8.10^{11}, N_{tot} \approx 7.10^{13}$$

4.Helium release due to bubble transportation by moving dislocations



Vb is the bubble velocity

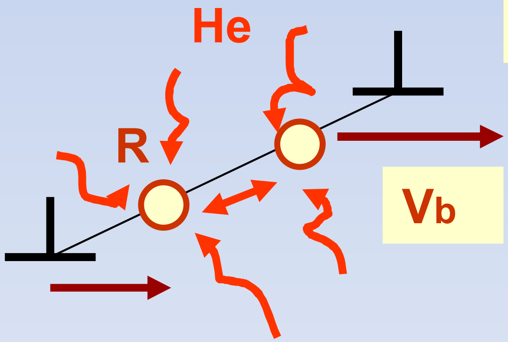
Lb is the distance between bubbles



$$\vec{V}_b = \frac{D_S}{8\pi kT}\left(\frac{b}{R}\right)^4 \vec{F}$$

$$F = \sigma b L_b$$

4.1 Nucleation and growth of helium bubbles on dislocations



1) Nucleation stage of bubbles on dislocations (τ_N)

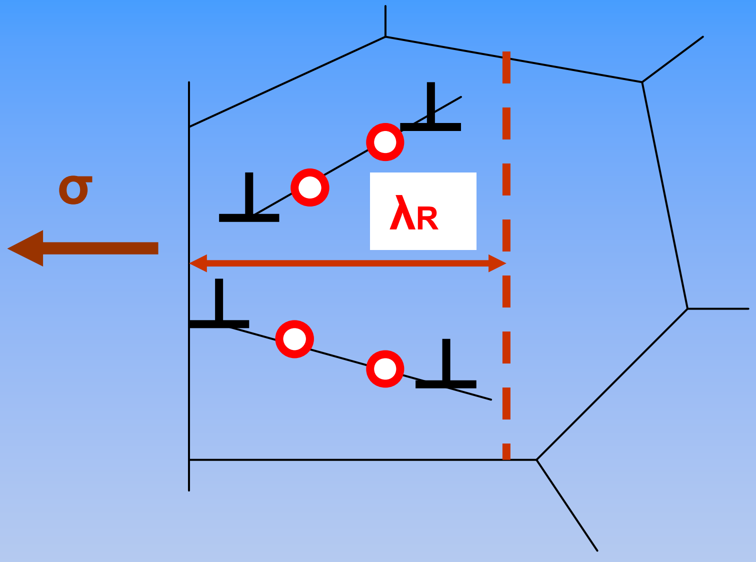
$$\tau_N \le \tau_d \approx \frac{R_d}{V_d}$$

$$L_b = L_b(t)$$

2) Bubble growth on dislocations (τ_G)

$$\tau_G \le \tau_d \approx \frac{R_d}{V_d}$$

$$R_b = R_b(t)$$



$$\lambda_R = \int_0^{\tau_R} V_b(t)\,dt$$

TR **is the time to rupture**

$$N_S = \frac{1}{32\pi kT}\frac{\sigma b^5 L_b}{C_{He}}\frac{D_S}{D^2_{He}}\frac{\tau_G^2 + \tau_R\tau_N}{\tau_G^2\tau_N}$$

C0 = 300 appm, T = 800 -1000K, L=10 µm, S0 =0.15cm2

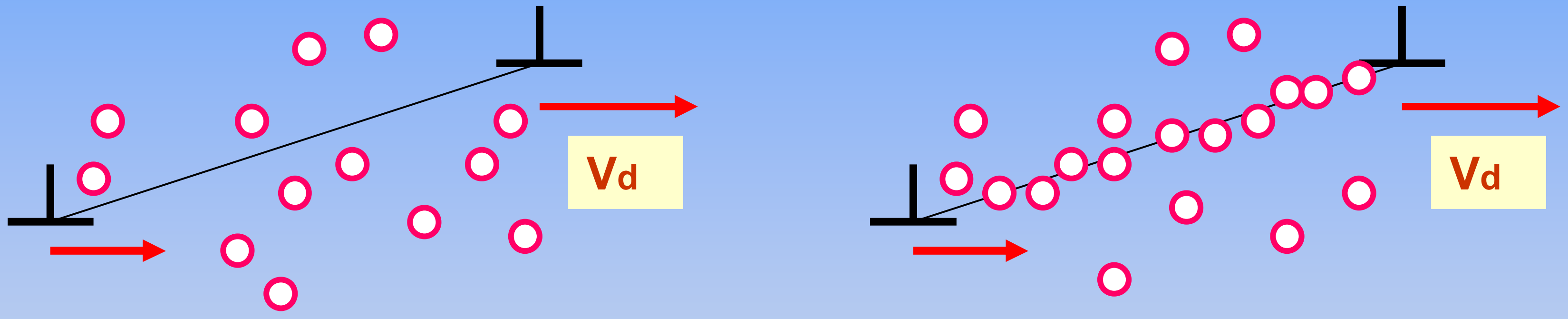
$$N_{tot} \propto \frac{\exp(-E/kT)}{kT}$$

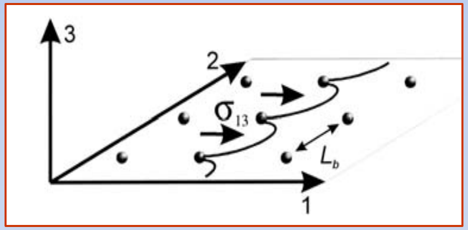
$$E = E_{mV} + E_{fV} - 2E_{mHe}$$

$$E_{mV} = 1eV, E_{fV} = 1.5eV, E_{mHe} = 0.008eV$$

$$N_{tot} \approx 4.10^{14} \div 3.10^{16}$$

4.2. Helium release due to sweeping of helium bubbles by moving dislocations





$$\tau_N \le \tau_d \approx \frac{R_d}{V_d}$$

$$N_S = \frac{D_S}{32\pi kT}\left(\frac{b}{R}\right)^4 \frac{\sigma b C_{He}}{R_d^2 C_B}\tau_R$$

$$N_{tot} \propto \frac{\exp(-E/kT)}{kT}$$

$$E = E_{mV} + E_{fV}$$

$$E_{mV} = 1eV, E_{fV} = 1.5eV$$

$$N_{tot} \approx 3.10^{13} \div 3.10^{15}$$

Summary

- Physical mechanisms of helium release during plastic deformation of V-alloys doped by helium atoms using tritium trick technique and cyclotron implantation were considered.
- The dislocation-dynamic model for helium release was determined in both limiting cases “slow” and “fast” helium atoms. The quantitative estimates for the case "fast" helium atoms (low deformation velocities, slow dislocations and saturation via tritium trick (helium atoms occupy interstitial sites)) at C_0=300 appm, T=800K and sample surface $S_0=0.15\text{cm}^2$ helium amount carrying by dislocation is $N=2\cdot10^{15}$, that is correlated with experimental data. In another limiting case ("slow" helium atoms) quantitative estimations show, that at C_0=300appm, ε=10%, L=10μm, So=0.15cm^2 the total amount of helium release is $N \sim 10^{13}$ and it is not correlated with observed experimental data.
- The mechanism related to sweep out of helium bubbles by moving dislocation is suggested. It was shown that this mechanism can contribute considerable part to helium release peaks formation.
- Temperature dependencies of total helium release for all of discussed mechanisms were analyzed. It was shown that in the model of dislocation dynamic diffusion total the helium amount come out to the surface has weak dependence on temperature

  $N \sim \ln(A/T))^{-1}$. The other discussed mechanisms have the following temperature dependence:

$$\boxed{N_{tot} \propto \frac{\exp\left(-E/kT\right)}{kT}}$$

where E is the effective helium energy migration $E_1 = E_{mv} + E_{fv} - 2E_{mHe}$, where E_{mv} is the vacancy energy migration, E_{mHe} is the helium atom energy migration, E_{fv} is the vacancy formation energy and in the case sweeping of helium bubbles by moving dislocations: $E_2=E_{mv}+E_{fv}$ .The obtained theoretical results have a good agreement with experimental data.

Thank you for your attention!