Chapter

Measurement of Vacancy Migration Energy by Using HVEM

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Abstract

Vacancy migration energy is a key factor for irradiation resistance of nuclear materials and also a fundamental parameter for modeling and should be experimentally calculated in advance. A new method together with a formula was developed for measuring the vacancy migration energy on high-voltage electron microscope (HVEM) from the temperature dependence of the growth speed of a dislocation loop in consideration of other sink effects including surface and grain boundary on point defects. Anti-noise property and the other characteristics of the three different methods have also been analyzed and discussed to help choose the appropriate method to measure the vacancy migration energy when in need in different situations.

Keywords: vacancy migration energy, in situ HVEM, measurement of E_m

1. Introduction

Fusion energy is one of the most promising carbon-free energy in the future. One problem limiting the development and application of fusion energy is the radiation damage of materials. Irradiation resistance of a material is determined by the motion and recombination of point defects (vacancy and interstitial) [1]. The motion and recombination of point defects are governed by the vacancy mobility at material service temperature which is always higher than the vacancy mobile temperature [1, 2]. Thus, vacancy migration energy is a critical factor for the ability of nuclear materials to resist radiation damage. Moreover, it is becoming a popular and an effective method to simulating the irradiation-induced microstructure changes to predict the mechanical properties of materials during irradiation with the development of computational materials. Vacancy migration energy is also a fundamental parameter for modeling and should be experimentally measured in advance.

Kiritani et al. have firstly proposed one method as early as the 1970s by experimentally measuring growth speed of interstitial dislocation loops at different irradiation temperatures to measure the motion of vacancies in iron by using HVEM [2, 3]. High-energy electron irradiation produces pure Frenkel point defect pairs, which is very beneficial to the fundamental research of point defect mobility. In combination with in situ heating sample holder, HVEM has been proven to be a powerful apparatus to investigate microstructural evolution and measure the vacancy migration energy under in situ high-energy electron irradiation. Since then, the method proposed by Kiritani et al. was often used to measure the vacancy migration energy of materials. The effects of impurities, helium, and hydrogen on

vacancy migration energy in pure Fe-based alloys, F82H and electron-beam-welded F82H joint, have been investigated by Hashimoto et al. [4–6]. The effect of deuterium on vacancy migration energy in Fe-10Cr alloy has also been investigated [7]. Point defect behavior in pure vanadium and its alloys were also analyzed under HVEM irradiation by using the method [8–10]. However, it is important to note that the method did not consider the effect of sample surface on the measurement of the vacancy migration energy. And, it is always very difficult to ensure that the observed loops are deep in the specimen (located so far apart from specimen surface) by HVEM stereo observation operation [11]. Thus, Wan et al. derived a new formula for calculation vacancy migration energy by considering the surface effect in the 1990s [11]. In this brilliant derivation, the effect of specimen surface was treated as a constant, and three data of growth rate at different irradiation temperatures were used once to numerically calculate the vacancy migration energy by iterated operation. This method considered the surface effect intrinsically, but iterated solution by using a computer is needed. This operation would produce two roots, in which one should choose the right one according to physical meaning. It is a little bit difficult to calculate and choose the right root. Probably for this reason, reference of using this numerical method is not many. Moreover, the effects of other sinks such as irradiation-induced small void, fine precipitates, and grain boundary on the growth speed of dislocation loops also needed to be considered when using HVEM to measure the vacancy migration energy.

In this chapter, other sinks such as surface, small void, precipitates, and grain boundary were taken into consideration to develop a new method for calculating vacancy migration energy according to the relationship of the reciprocal of irradiation temperature and growth speed of dislocation loops. An influential factor relating to the effects of other sinks was also presented in this new method. In addition, the formula derived by Wan et al. has also been rediscussed to avoid one root and help to choose the right root, which may encourage a broader range of applications of this numerical method. The characteristic of these three methods is discussed to help choose the appropriate method to measure the vacancy migration energy when in need in different situations. In addition, the motion interstitial is also important and could be measured by using HVEM [12, 13]. In this chapter, however, we only discussed the mobility of vacancy because vacancy moves much slower than that of interstitial, and the recombination of vacancies and interstitial defects is governed by the vacancy mobility at material service temperature which is higher than vacancy mobile temperature.

2. The calculation method

2.1 Linear method

This method was reported by Kiritani et al. [2] and Tabata et al. [14] in which several factors affecting the migration energy were discussed in detail. According to their analysis, the variations of the concentrations of interstitial atoms (C_i) and lattice vacancies (C_v) with the point defect mobility (M) at high temperature (at which vacancies are highly mobile) are given as follows:

$$\frac{dC_i}{dt} = P - Z_{iv}(M_i + M_v)C_iC_v - Z_{iL}M_iC_{sL}C_i - M_iC_{si}C_i \quad (1)$$

and

$$\frac{dC_v}{dt} = P - Z_{iv}(M_i + M_v)C_iC_v - Z_{vL}M_vC_{sL}C_v - M_vC_{sv}C_v \tag{2}$$

where Z_{iv}, Z_L, and C_s denote the recombination coefficient, the number of reaction sites of dislocation loops and point defects, and concentration of sinks, respectively. And, t denotes the time. First term P is the production rate of free Frenkel pairs induced by HVEM. The second term is the mutual annihilation rate between interstitials and vacancies with the mutual annihilation cross-section of Z_{iv}. The third terms are the annihilation rate of each kind of point defect to dislocation loops whose concentration of atomic sites as sinks is C_{sL} and with absorption cross-sections Z_{iL} and Z_{vL} at each site for each point defect. The last terms are the annihilation at the surface sink. When a steady state of point defect concentrations is established, there is:

$$\frac{dC_i}{dt} = \frac{dC_v}{dt} = 0 \tag{3}$$

Then, both Eqs. (1) and (2) are equal to zero, and one can obtain the following equation:

$$(Z_{iL}C_{sL} + C_{si})M_iC_i = (Z_{vL}C_{sL} + C_{sv})M_vC_v \tag{4}$$

The most dominant terms of the point defect annihilation are the second terms in Eqs. (1) and (2), at least for the "thick-foil" case in which the last terms in the equations never become dominant. Then one can obtain the following, under the condition of $M_i \gg M_v$:

$$P = Z_{iv}M_iC_iC_v \tag{5}$$

Using Eqs. (4) and (5), the following equation could be obtained:

$$M_vC_v = \beta M_iC_i = \frac{\beta P}{Z_{iv}C_v} = \sqrt{\frac{\beta P M_v}{Z_{iv}}} \tag{6}$$

where $\beta = (Z_{iL}C_{sL} + C_{si})/(Z_{vL}C_{sL} + C_{sv})$. Since C_{si} and C_{sv} are considered to be equal to each other and stay constant as long as the loop remains at the same fixed position in a specimen foil, the value β is thought to be slightly larger than unity because of the slightly larger capture cross-section Z_{iL} for interstitial than that for vacancy, Z_{vL}, at a dislocation loop and can be taken as constant (at least at a fixed temperature) though it varies slowly with the increase of C_{sL} by the growth of the dislocation loops [2].

The growth speed of interstitial loop of size R is expressed by the arrival rate to the loop of interstitial atoms in excess of vacancies and is:

$$\frac{\mathrm{dR}}{\mathrm{dt}} = a(Z_{iL}M_iC_i - Z_{vL}M_vC_v) = a\left(\frac{\frac{Z_{iL}}{\sqrt{\beta}} - \sqrt{\beta}Z_{vL}}{\sqrt{z_{iv}}}\right)\sqrt{P}\sqrt{M_v} \tag{7}$$

where a is the increase of loop size by the absorption of one point defect per one site on the dislocation [2]. $Z_{iL}M_iC_i$ and $Z_{vL}M_vC_v$ are the ensemble of point defect fluxes captured by the loop. In order to reduce the effect of loop's size, the loops with same/similar initial size should be selected during experimental operation, which can be done relatively easily. Then, the equation can be written as:

$$\frac{dR}{dt} = C \cdot \exp\left(\frac{-E_m^v}{2kT}\right) \tag{8}$$

where k is the Boltzmann constant and C is an experimental constant. The above equation can be rewritten as:

$$\ln\left(\frac{dR}{dt}\right) = lnC - \frac{E_m^v}{2kT} \tag{9}$$

Using this equation, the vacancy migration energy can therefore be obtained from the slope of a linear relationship between the logarithm of the growth rate of dislocation loops and the inverse of temperature. Here, we called this method "linear method."

2.2 Numerical method

Using the "linear method" with Eq. (9), the vacancy migration energy can be calculated simply. However, the position of the dislocation loop must be deep in the thick foil to ensure the surface effect could be avoided. This makes the experiment more complex and difficult. Considering the surface effect of the sample, another brilliant derivation was developed by not avoiding the third and fourth terms of Eqs. (1) and (2) by Wan et al. [11].

When the point defect concentration is in a steady state, there is $dC_i/dt = dC_v/dt = 0$. And one can obtain an equation under the condition of $M_i \gg M_v$:

$$P = Z_{iv}M_iC_iC_v + Z_{vL}M_vC_{sL}C_v + M_vC_{sv}C_v = \frac{Z_{iv}}{\beta M_v}(M_vC_v)^2 + (Z_{vL}C_{sL} + C_{sv})M_vC_v \tag{10}$$

The former equation can be written as:

$$\frac{A_1}{M_v}(M_vC_v)^2 + B_1M_vC_v - P = 0 \tag{11}$$

where A_1 and B_1 are constant. The root of this equation is:

$$M_vC_v = \left(-B_1 \pm \sqrt{B_1^2 + \frac{4PA_1}{M_v}}\right)\frac{M_v}{2A_1} \tag{12}$$

Substituting Eq. (12) into Eq. (7), one can obtain:

$$\frac{\mathrm{dR}}{\mathrm{dt}} = a(Z_{iL}M_iC_i - Z_{vL}M_vC_v) = a\left(\frac{Z_{iL}}{\beta} - Z_{vL}\right)M_vC_v = \left(B_2 \pm \sqrt{B_2^2 + \frac{A_2}{M_v}}\right)M_v \tag{13}$$

where A_2 and B_2 are constant. This equation can be changed to be:

$$exp\left(\frac{E_m}{kT}\right)\left(\frac{dR}{dt}\right)^2 - B_3\left(\frac{dR}{dt}\right) - A_3 = 0 \tag{14}$$

Letting dR/dt = V, the above equation can be expressed as:

$$exp\left(\frac{E_m}{kT}\right)V^2 - B_3V - A_3 = 0 \tag{15}$$

By HVEM observation, V_1, V_2, and V_3 at temperatures T_1, T_2, and T_3 can be obtained, respectively. Using these data in Eq. (15) and getting rid of the constant, there is:

$$\frac{V_1 - V_2}{V_2 - V_3} = \frac{V_1^2 exp\left(\frac{E_m}{kT_1}\right) - V_2^2 exp\left(\frac{E_m}{kT_2}\right)}{V_2^2 exp\left(\frac{E_m}{kT_2}\right) - V_3^2 exp\left(\frac{E_m}{kT_3}\right)} \tag{16}$$

Letting $(V_1 - V_2)/(V_2 - V_3) = V_0 > 0$ and substituting it in Eq. (16), the vacancy migration energy is given as follows:

$$a_1 \cdot \exp\left(E_m \cdot b_1\right) + a_2 \cdot \exp\left(E_m \cdot b_2\right) - 1 = 0 \tag{17}$$

where

$$a_1 = \frac{V_1^2}{(1+V_0)V_2^2}, a_2 = \frac{V_0V_3^2}{(1+V_0)V_2^2}, b_1 = \frac{1}{k}\left(\frac{1}{T_1} - \frac{1}{T_2}\right), \quad b_2 = \frac{1}{k}\left(\frac{1}{T_3} - \frac{1}{T_2}\right)$$

and where k is the Boltzmann constant. Eq. (17) can be solved by using a computer. A Python program example for solving Eq. (17) is given in the Appendix. According to Eq. (17), two mathematical results would be obtained. In this case it is necessary to select one of these two results by the physical meaning. Sometimes, one will have a little difficulty in choosing the correct result. Probably for this reason, the application of this method had been limited.

The derivation was discussed here again to help select the result of Eq. (17). Two roots were induced by the Eq. (11) firstly. We can avoid one root directly in Eq. (12) by the physical meaning:

$$2A_1C_v > 0$$

where $A_1 = Z_{iv}/\beta > 0$, C_v is the concentration of the vacancy. So, Eq. (12) could be rewritten as:

$$M_vC_v = \left(-B_1 + \sqrt{B_1^2 + \frac{4PA_1}{M_v}}\right)\frac{M_v}{2A_1} \tag{18}$$

The Eq. (13) can also be changed to:

$$\frac{dR}{dt} = a(Z_{iL}M_iC_i - Z_{vL}M_vC_v) = \left(B_2 + \sqrt{B_2^2 + \frac{A_2}{M_v}}\right)M_v \tag{19}$$

There should be only one root for E_m in the Eq. (15) in which A_3 and B_3 are constant. Thus, one knows to choose the big one of the two results from Eq. (17). Only one result will be obtained. This may encourage a broader range of applications of this method as it considers the surface effect intrinsically. We called this method "numerical method" here because of numerical calculating of the vacancy migration energy by iterated operation [15].

2.3 Nonlinear method

Using linear method, the vacancy migration energy could be obtained simply with no consideration of the surface effect. In order to ensure the surface effect could be avoided, however, the position of the dislocation loop must be deep which is difficult sometimes and will make the HVEM experiment more complex. Considering other sink effects such as surface, small void, precipitates, and grain boundary, some terms were added in Eqs. (1) and (2):

$$\frac{dC_i}{dt} = P - Z_{iv}(M_i + M_v)C_iC_v - Z_{iL}M_iC_{sL}C_i - Z_{io}M_iC_{so}C_i - Z_{iP}M_iC_{sp}C_i - Z_{iB}M_iC_{sB}C_i - M_iC_{si}C_i \tag{20}$$

$$\frac{dC_v}{dt} = P - Z_{iv}(M_i + M_v)C_iC_v - Z_{vL}M_vC_{sL}C_v - Z_{vo}M_vC_{so}C_v - Z_{vP}M_vC_{sp}C_v - Z_{vB}M_vC_{sB}C_v - M_vC_{sv}C_v \tag{21}$$

where Z_{iv}, Z_L, and C_s denote the recombination coefficient, the number of reaction sites of dislocation loops, and point defects and density of sinks, respectively. The first term P is the production rate of free Frenkel pairs induced by HVEM. The second term is the mutual annihilation between interstitials and vacancies. The third terms are the annihilation rate of each kind of point defect to dislocation loops whose concentration of atomic sites as sinks is C_{sL} and with absorption cross-sections Z_{iL} and Z_{vL} at each site for each point defect. The fourth, fifth, and sixth terms are the ensemble of annihilation of each kind of point defect to void, precipitates, and grain boundary, respectively. It is worth noting that these three kinds of sinks mean a very small one or inconspicuous one which could not be observed by HVTEM at the same magnification times as observing the whole loop. One can avoid it directly during the TEM observation if the void or precipitates are big enough, which will not be discussed here. The seventh terms express the escape of point defects to the surface sink. Under the condition of $M_i >> M_v$ and the steady state of point defect concentrations ($\frac{dC_i}{dt} = \frac{dC_v}{dt} = 0$), Eqs. (20) and (21) can be written as:

$$P = Z_{iv}M_iC_iC_v + Z_{vL}M_vC_{iL}C_v + Z_{vo}M_vC_{so}C_v + Z_{vP}M_vC_{sP}C_v + Z_{vB}M_vC_{sB}C_v + M_vC_{sv}C_v \tag{22}$$

Then, there is:

$$\frac{Z_{iv}}{\beta M_v}(M_vC_v)^2 + \left(Z_{vL}C_{sL} + Z_{vo}C_{so} + Z_{vp}C_{sP} + Z_{vB}C_{sB} + C_{sv}\right)M_vC_v - P = 0 \tag{23}$$

where $\beta = (Z_{iL}C_{sL} + Z_{io}C_{so} + Z_{iP}C_{sP} + Z_{iB}C_{sB} + C_{si}) / (Z_{vL}C_{sL} + Z_{vo}C_{so} + Z_{vP}C_{sP} + Z_{vB}C_{sB} + C_{sv})$.

Set $a_1 = \frac{Z_{iv}}{\beta}$ and $b_1 = Z_{vL}C_{sL} + Z_{vo}C_{so} + Z_{vP}C_{sP} + Z_{vB}C_{sB} + C_{sv}$. According to the physical meaning, a_1 and b_1 are constant larger than zero. The above equation can be written as:

$$\frac{a_1}{M_v}(M_vC_v)^2 + b_1M_vC_v - P = 0 \tag{24}$$

The root of Eq. (24) is:

$$M_vC_v = \left(-b_1 \pm \sqrt{b_1^2 + \frac{4Pa_1}{M_v}}\right)\frac{M_v}{2a_1} \tag{25}$$

According to the physical meaning, M_vC_v should be larger than zero, while $\left(-b_1 - \sqrt{b_1^2 + \frac{4Pa_1}{M_v}}\right)\frac{M_v}{2a_1} < 0$. Anyway, substituting Eq. (25) into Eq. (7), the following equation can be obtained:

$$\frac{\mathrm{dr}}{\mathrm{dt}} = a\left(\frac{Z_{iL}}{\beta} - Z_{vL}\right)M_vC_v = \left(b_2 \pm \sqrt{b_2^2 + \frac{a_2}{M_v}}\right)M_v \tag{26}$$

where a is the change of loop radius by the absorption of one point defect per one site on the dislocation [2].

$\left(\frac{Z_{iL}}{\beta} - Z_{vL}\right) \approx (Z_{iL} - Z_{vL}) = L_{bias}$, thus, $a_2 = \frac{a^2PL_{bias}^2}{a_1}$ and $b_2 = \frac{-b_1 a L_{bias}}{2a_1}$

Eq. (26) can be changed into:

$$exp\left(\frac{E_m}{kT}\right)\left(\frac{dr}{dt}\right)^2 - b_3\left(\frac{dr}{dt}\right) - a_3 = 0 \tag{27}$$

where $a_3 = 1/4a_2$, $b_3 = b_2$. The above equation can be written as:

$$exp\left(\frac{E_m}{kT}\right) = a_3\left(\frac{dt}{dr}\right)^2 + b_3\left(\frac{dt}{dr}\right) \tag{28}$$

As a_3, b_3 and $\frac{b_3^2}{4a_3} = \frac{b_2^2}{a_2} = \frac{b_1^2}{4Pa_1}$ are constant. There is a constant d to hold the following equation:

$$d * exp\left(\frac{E_m}{kT}\right) = a_3\left(\frac{dt}{dr} + \frac{b_3}{2a_3}\right)^2 \tag{29}$$

From the above equation, one can obtain:

$$\frac{1}{T} = \frac{2k}{E_m} * \ln\left(\frac{dt}{dr} + B_1\right) + C_1 \tag{30}$$

where $B_1 = b_3/2a_3$ and C_1 is constant. By HVEM observation and getting dt/dr [1/(dr/dt)] data at different temperatures, the E_m can be obtained by this equation. In order to plot easily, the equation can be rewritten as:

$$\frac{1000}{T} = \mathrm{A} * \ln\left(\frac{1}{(dr/dt)} + B\right) + C \tag{31}$$

Note: $A = 2\,k^*1000/E_m$, $B = -b_1/(a^*P)$ is a negative constant relating to total effects of all other sinks. Thus, from the function of 1/(dr/dt) and 1/T, the E_m can be obtained by plotting the curve according to Eq. (31).

3. Discussion

Measurement of vacancy motion in solid state materials is a challenging work. There are not so many experimental methods. In situ HVEM has been proven to be one of the powerful tools to obtain vacancy migration energy by measuring the temperature dependence of the growth speed of a dislocation loop during electron irradiation. A reasonable phenomenological model of the loop growth could be selected and applied to extract the vacancy migration energy from the experimental

data. Kiritani et al. firstly proposed one linear model to calculate the vacancy migration energy. Then, Wan et al. derived a new formula by considering the surface effect. In this chapter, a new nonlinear model was developed by considering the other sink effects such as surface, small void, small precipitates, and grain boundary, and the numerical method was rediscussed. When the measured experimental data are ideal, not affected by the surface or other defect sinks, the vacancy migration energy value calculated by the three methods should be the same. One experimental example for calculating the vacancy migration energy by using the three methods was given here. The sample was Fe-10Cr model alloy which was pre-implanted by He and H ion sequentially. Then electron irradiation and in situ observation were carried out in HVEM at 573, 673, and 773 K. At a corresponding temperature, the growth rates of dislocation loop were measured [15]. But, the ln (dR/dt) and 1/T calculated from the experimental data were not strict linear that means there may be influences from the sample surface or other sinks. Thus, three assumed ideal values of the growth rate which are close to the three experimental values were selected to test the three methods, which are about 1.1 nm/min at 573 K, 3.5 nm/min at 673 K, and 8.1 nm/min at 773 K, respectively. According to these values, the ln(dR/dt) and 1/T followed a strict linear relationship, which means an ideal situation without the effect of other sinks. Then, the three methods were used to calculate the vacancy migration energy in this ideal case, and the results were shown in **Figure 1**. **Figure 1(a)** showed the result calculated by the linear method where blue squares are the experimental data and red pentagrams are the ideal values. The result calculated by the numerical method was shown in **Figure 1(b)**; the solving process example of the Eq. (17) was given in the Appendix. **Figure 1(c)** showed the result calculated by the nonlinear method where the horizontal axis

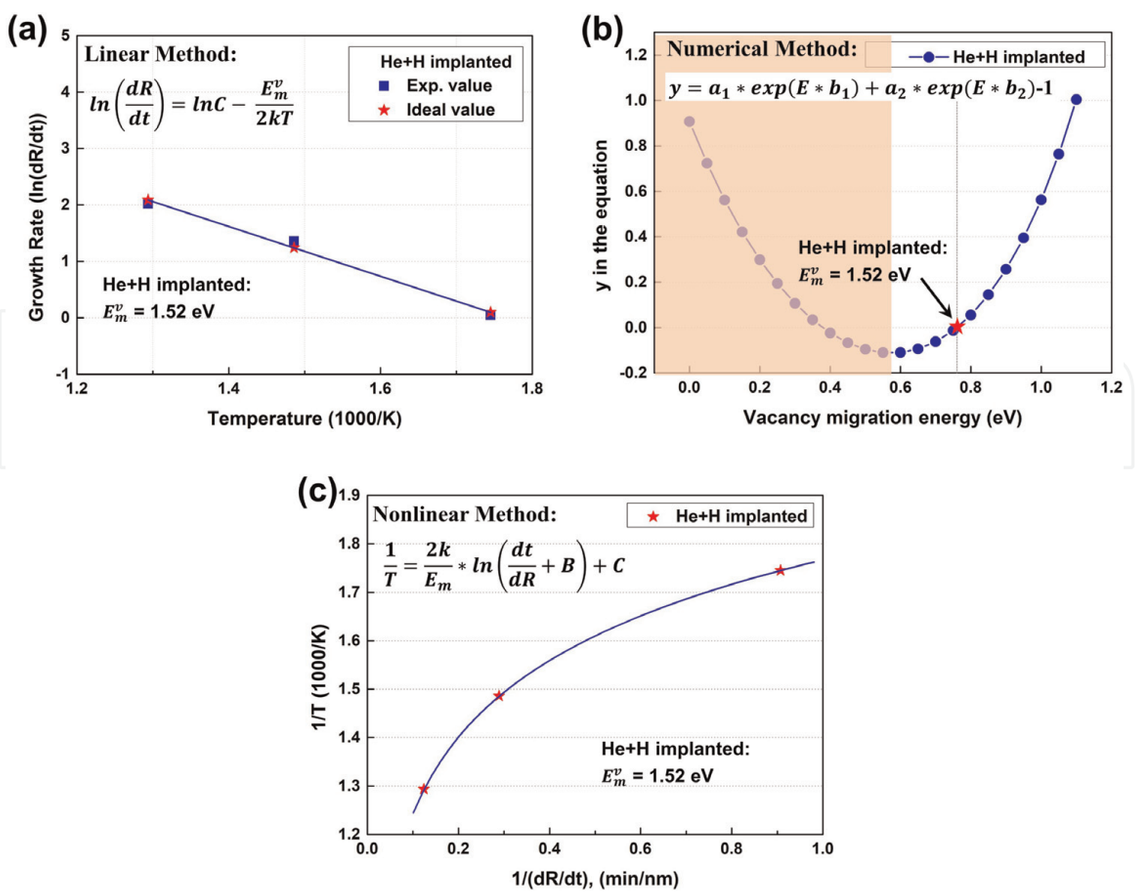

Figure 1.
Measurement of vacancy migration energy in sequential-(He+H) ion implanted Fe-10Cr samples according to the ideal values by using linear method (a), numerical method (b), and nonlinear method (c), respectively.

Methods	Considering surface effect	Considering other sinks effect	Anti-noise property
Linear method	No	No	Very good
Numerical method	Yes	No	—
Nonlinear method	Yes	Yes	Good

Table 1.
The characteristics of three methods for measuring vacancy migration energy.

represents the inverse of the growth rate and the vertical axis represents the inverse of temperature. These results indicated that the vacancy migration energy value calculated by the three methods according to ideal values in He+H pre-implanted Fe-10Cr sample was the same which was about 1.52 eV, while the vacancy migration energy values calculated by a different method according to the experimental data were different because of the different characteristics of the method. The characteristics of three methods for measuring vacancy migration energy were listed in **Table 1**.

In addition, if the linear fitting degree is larger than 0.9 which means the effect of other sinks was not dominated, linear model was preferred to fitting the experimental data and obtaining the value of vacancy migration energy because it is very simple. Otherwise, nonlinear model or numerical method should be used in considering the surface effect and other sink effect intrinsically. And, the overall influence of other sinks was also given as an influence factor (B) in the nonlinear model. It is worth to note that the "nonlinear method" has one more parameter than "linear method," which means there is a bigger possibility for overfitting problem to arise. Thus, one should notice that parameter B should be negative according to Eq. (31) to avoid the overfitting problem. Another thing which needs to be noted is that $M_i >> M_v$ is appropriate for pure metals, but $M_v > M_i$ may exist for some alloys [11, 16, 17]. The anti-noise property and the result reliability of different methods were also discussed in Ref. [18] and listed in **Table 1**. Then, one can choose an appropriate method to measure the vacancy migration energy according to the anti-noise property, result reliability, and other characteristics of the three different methods.

4. Summary

In summary, the methods to measure the vacancy migration energy by using HVEM were described and discussed in this chapter. Considering other sinks effects, a new nonlinear method was developed to measure vacancy migration energy according to the relationship of the reciprocal of irradiation temperature and growth speed of dislocation loops. Meanwhile, an influential factor relating to the effects of other sinks was also presented. The characteristics of three methods for measuring vacancy migration energy were also discussed in detail, which can help to select the appropriate method to measure the vacancy migration energy in different situations.

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Appendix

Python program example (He+H implanted sample for example) for solving Eq. (17) is given here. Two methods were tried to solve Eq. (17). One is Newton iteration method and another is directly plotting the curve. Here we paste the program to illustrate the solving of Eq. (17) by directly plotting, which may be the simplest and most effective method.

```
#Python 3.6
#Filename: Cal Em by using Numerical Method plot curve of Em

import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

print('-------------------------------------------')
print('Import the growth rate data of He+H implantation...')

(t,v)=np.loadtxt('.\\loop growth rate_He+H.txt', skiprows=1, unpack=True)

print('T(K)',' V(nm/min)')
print(t[0],v[0])
print(t[1],v[1])
print(t[2],v[2])

v0=(v[0]-v[1])/(v[1]-v[2])
v0=float('%.5f'%v0)
print('\nV0 is:',v0)

a1=(v[0]*v[0])/((1+v0)*v[1]*v[1])
a1=float('%.5f'%a1)
a2=(v0*v[2]*v[2])/((1+v0)*v[1]*v[1])
a2=float('%.5f'%a2)
b1=100000*(1/t[0]-1/t[1])/8.6
b1=float('%.5f'%b1)
b2=100000*(1/t[2]-1/t[1])/8.6
b2=float('%.5f'%b2)

print('\ny=a1*exp(E*b1)+a2*exp(E*b2)-1')
print('a1   ','b1   ','a2   ','b2')
print(a1,b1,a2,b2)

#Plotting of Em of He+H-implanted sample
x=np.arange(0,1.1,0.000005)

#y=a1*exp(x*b1)+a2*exp(x*b2)-1, is not available here, use y=y1+y2
y1=a1*np.exp(x*b1)
```

```
    y2=a2*np.exp(x*b2)-1
    y=y1+y2

    i=len(x)-1
    while y[i]>0.00001:
        i=i-1
    else:
        print('Em:',2*x[i]) #M. Kiritani, H. Takata, K. Moriyama, et al., Philos. Mag. A,
40 (1979) 779-802.
        print('y:',y[i])

    He+H_data={'y=a1*exp(x*b1)+a2*exp(x*b2)-1':y,
               'Em':x}
    df1=pd.DataFrame(He+H_data)
    df1.to_csv('.\\He+H_data.csv')

    plot1=plt.plot(x,y,'r',label='He+H implanted')

    plt.xlabel('E')
    plt.ylabel('y in the equation')
    plt.legend(loc=2)

    plt.show()
    plt.savefig('p1.png')
```

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