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Analysis of spinodal decomposition in Fe-32 and 40 at.% Cr alloys using phase field method based on linear and nonlinear Cahn-Hilliard equations

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ABSTRACT: Spinodal decomposition was studied during aging of Fe-Cr alloys by means of the numerical solution of the linear and nonlinear Cahn-Hilliard differential partial equations using the explicit finite difference method. Results of the numerical simulation permitted to describe appropriately the mechanism, morphology and kinetics of phase decomposition during the isothermal aging of these alloys. The growth kinetics of phase decomposition was observed to occur very slowly during the early stages of aging and it increased considerably as the aging progressed. The nonlinear equation was observed to be more suitable for describing the early stages of spinodal decomposition than the linear one.

KEYWORDS: Cahn-Hilliard equations; Fe-Cr alloys; Phase field method; Spinodal decomposition

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RESUMEN: *Análisis de la descomposición espinodal en aleaciones Fe-32 y 40 %at. Cr utilizando el método de campo de fases basado en las ecuaciones lineal y no lineal de Cahn y Hilliard.* La descomposición espinodal se estudió durante el envejecido de aleaciones Fe-Cr mediante la solución numérica de las ecuaciones diferenciales parciales lineal y no linear de Cahn y Hilliard usando el método de diferencias finito explícito. Los resultados de la simulación numérica permitieron describir apropiadamente el mecanismo, morfología y cinética de la descomposición de fases durante el envejecido isotérmico de estas aleaciones. La cinética de crecimiento de la descomposición de fases ocurrió muy lentamente durante las primeras etapas de envejecido, y se incrementó considerablemente con el tiempo de envejecido. La ecuación no lineal parece ser más apropiada para describir las primeras etapas de la descomposición espinodal que la ecuación lineal.

PALABRAS CLAVE: Aleaciones Fe-Cr; Descomposición espinodal; Ecuaciones de Cahn y Hilliard; Método de campo de fases

1. INTRODUCTION

The ferritic and martensitic stainless steels are mainly based on the Fe-Cr alloy system, and thus these binary alloys are considered a model to study the phase transformations in this type of steels (Danoix and Auger, 2000; Senninger *et al.*, 2014). The corrosion resistance and their excellent mechanical properties are fundamental in Fe-Cr alloys with Cr contents higher than 12 at.% in order to be used as structural materials in the chemical, petrochemical and power generation industries. Nevertheless, the mechanical properties can be reduced in Fe-Cr alloys because of heating at temperatures between 280 and 500 °C even for short times. This phenomenon is known as 475 °C-embrittlement and it has been associated with the phase decomposition of the Fe-Cr solid solution into a mixture of bcc Fe-rich (α) and Cr-rich (α') phases via either the nucleation and growth or spinodal decomposition mechanisms during aging at these temperatures (La Salle and Schwartz, 1986; Terentyev *et al.*, 2008; Tomoaki *et al.*, 2015).

The phase decomposition of Fe-Cr alloys has been reported to occur by the nucleation and growth mechanism in Cr contents between 12 and 30 at.% (Bonny *et al.*, 2008; Dongsheng *et al.*, 2014). In contrast, the phase decomposition was reported recently (Jing *et al.*, 2013) to take place via spinodal decomposition during aging of Fe-Cr alloys with Cr contents between 25 and 36 wt.% Cr.

The phase decomposition of Fe-Cr alloys has been studied using different experimental techniques, as shown above. Recently, the application of numerical methods to the analysis of phase transformations such as the phase field method has permitted to study the phase decomposition process of aged and neutron-irradiated Fe-Cr alloys. This caused hardening and embrittlement at temperatures between 300 and 500 °C (Martínez *et al.*, 2012; Dubiel and Zukrowski, 2013; Malerba *et al.*, 2013).

The phase field method has also proved to be a powerful tool to analyze the spinodal decomposition process in different alloys (Honjo and Saito, 2000; Soriano *et al.*, 2010). The phase field model can be based on the solution of the nonlinear Cahn-Hilliard equation (Cahn and Hilliard, 1958), but it is also possible to employ the linear one which seems to be useful at the early stages of spinodal decomposition (Cahn and Hilliard, 1971).

Thus the purpose of present work is to apply both solutions of linear and nonlinear equations for analyzing the spinodal decomposition process in isothermally aged Fe-32 and 40 at.% Cr alloys, as well as the comparison of simulated microstructure evolution to those obtained by High-Resolution (HR) transmission electron microscope of the aged specimens.

2. EXPERIMENTAL DETAILS

Fe-32 and 40 at.% Cr alloys were prepared by melting of pure iron (99.99%) and Cr (99.99%) metals in an electric-arc furnace under an argon atmosphere. The as-cast alloys were homogenized at 1100 °C for 240 h. Both alloy specimens were encapsulated in quartz tubes under an argon atmosphere and then solution treated at 1000 °C for 2 h and subsequently quenched in ice-water. These specimens were aged at 470 and 500 °C for times from 10 to 500 h in a tubular electric furnace. TEM specimens were prepared using a twin-jet electropolisher with a chemical solution composed of 33 vol. % HNO_3 in CH_3-OH at a temperature of about -35° C. The aged specimens were observed with a JEOL JEM 2200FS HR-TEM at 300 kV.

3. NUMERICAL PROCEDURE

The phase decomposition simulation was based on a numerical solution of the following linear and nonlinear Cahn-Hilliard equation (Honjo and Saito, 2000), Eqs. (1) and (2).

$$\frac{\partial c\ (x,t)}{\partial t} = M\,\nabla^2 \left(\frac{\partial f_o(c)}{\partial c} - K\,\nabla^2 c \right) \tag{1}$$

$$\frac{\partial c\ (x,t)}{\partial t} = M\left[\left(\frac{\partial^2 f_o(c)}{\partial c^2} + 2\eta^2 Y \right) \nabla^2 c \ - 2K\,\nabla^4 c \right] \tag{2}$$

where $c(x,\ t)$ is the concentration as a function of distance x and time t, M is the atomic mobility, f_o is the local free energy, and K is the gradient energy coefficient. Y is an elastic constant. The parameter η is the lattice mismatch between the decomposed phases.

The local energy f_o was defined assuming a regular solution model expressed by

$$\begin{aligned} f_o = {} & f_{Cr} c_{Cr} + f_{Fe} c_{Fe} + \Omega_{Fe-Cr} c_{Cr} c_{Fe} \\ & + RT\left[c_{Cr} \ln c_{Cr} + c_{Fe} \ln c_{Fe} \right] \end{aligned} \tag{3}$$

where R is the gas constant, T is the absolute temperature. f_{Cr} and f_{Fe} are the molar free energy of pure Cr and Fe, respectively, and $\Omega_{Fe\text{-}Cr}$ is the interaction parameter.

The atomic mobility M is associated with the interdiffusion coefficient $\bar{D}$ as follows (Honjo and Saito, 2000):

$$\bar{D} = M\left(\frac{\partial^2 f_o}{\partial c_i^2} \right) \tag{4}$$

The interdiffusion coefficient $\bar{D}$ was defined (Hilliard, 1970) by the following expression

$$\bar{D} = D_{Fe}\, c_{Cr} + \left(1 - c_{Cr}\right) D_{Cr} \tag{5}$$

The gradient energy coefficient k was defined as proposed by Hilliard (1970)

$$k = \left(\frac{2}{3}\right) h_{0.5}^{M}\, r_0^2 \tag{6}$$

where, $h_{0.5}^{M}$ is the heat of mixing per unit volume at $c = 0.5$ and r_o is the nearest-neighbor distance. The heat of mixing h^M was determined according to the following equation (Honjo and Saito, 2000):

$$h^M = c_{Cr} c_{Fe}\, \Omega_{Fe-Cr} \tag{7}$$

The elastic energy was introduced into Eqs. (1 and 2), according to the following definition proposed by Hilliard (1970):

$$f_{el} = A \int \eta^2\, Y \left(c - c_0\right)^2 dx \tag{8}$$

where A is the cross-sectional area, Y an elastic constant defined by the elastic stiffness constants, c_{11}, c_{12} and c_{44} for the Cr-rich and Fe-rich phases. The parameter η is equal to $dlna/dc$ and a is the lattice parameter. The Y value can be assumed similar to that corresponding to an isotropic material (Dieter, 1988) and it is given by

$$Y = c_{11} + c_{12} - 2\left(\frac{c_{12}^2}{c_{11}}\right) \tag{9}$$

The elastic constants, $c_{ij,}$ were assumed to follow the subsequent relation:

$$c_{ij} = c_{ij}^{Cr}\, c_{Cr} + c_{ij}^{Fe}\, \left(1 - c_{Cr}\right) \tag{10}$$

The lattice, diffusion, thermodynamic and elastic constants for the microstructural simulation in Fe-Cr alloys were taken from references (Pearson, 1958; Hilliard, 1970; Dieter, 1988; Mehrer, 1990; Honjo and Saito, 2000) and they are shown in Table 1. The simulation of phase decomposition was carried out using the explicit finite difference method with 101 x 101 and 201 x 201 points-square grits with a mesh size of 0.1 and 0.25 nm and a time-step size up to 10 s. This simulation was performed for the Fe-32 and 40 at.% Cr alloys aged at 470 and 500 °C for times from 0 to 1000 h. It is important to mention that the initial composition modulation corresponding to the solution treated sample was calculated using a random-number generator (Honjo and Saito, 2000).

4. RESULTS

4.1. Concentration profiles of the aged alloys

The plots of Cr concentration versus distance, concentration profiles, for the Fe-32 and 40at.% Cr alloy aged at 470 °C for different times are shown in Fig. 1 (a–b) for the solution of nonlinear and linear Cahn-Hilliard equations, respectively. Both concentration profiles indicates clearly that the supersaturated solid solution decomposed spinodally into a mix of Cr-rich α_1 and Fe-rich α_2 phases since the modulation amplitude increases as the aging time increases. The modulation amplitude of the Fe-40at.% Cr alloy is higher than that corresponding to the other alloy composition for the same aging time at the early stages of aging since this composition is located closer to the center of miscibility gap and thus it has a higher driving force for the spinodal decomposition (Cahn and Hilliard, 1971). The modulation amplitude of both alloy compositions is almost the same for aging times longer than 500 h since the decomposed phase composition is close to the equilibrium line, miscibility gap.

TABLE 1. Lattice, diffusion, elastic and thermodynamic constants

Parameter	Values
Lattice Parameter a (nm)	a=0.2866 (Pearson, 1958)
Diffusion coefficient D ($cm^2\ s^{-1}$)	D_{Fe}=1.2 exp (−294000 J mol^{-1})/RT (Mehrer, 1990) D_{Cr}=0.2 exp (−308000 J mol^{-1})/RT
$\Omega_{Fe\text{-}Cr}$ (J mol^{-1})	(18600.0+0.1T) (Honjo and Saito, 2000)
c_{ij} (J m^{-3}) Fe Cr	(Dieter, 1988) c_{11}=23.10×10^{10} c_{12}=13.54×10^{10} c_{44}=11.78×10^{10} c_{11}=35.00×10^{10} c_{12}=67.80×10^{10} c_{44}=10.08×10^{10}
η	0.00614 (Pearson, 1958)

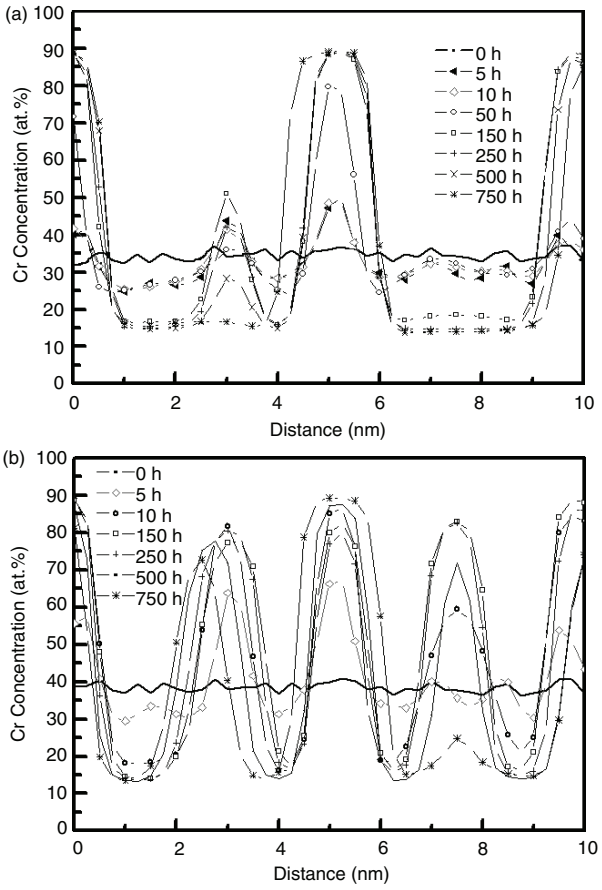

FIGURE 1. Concentration profiles of the: (a) Fe-32 and (b) 40 at.% Cr alloys aged at 470 °C for different times using the nonlinear equation.

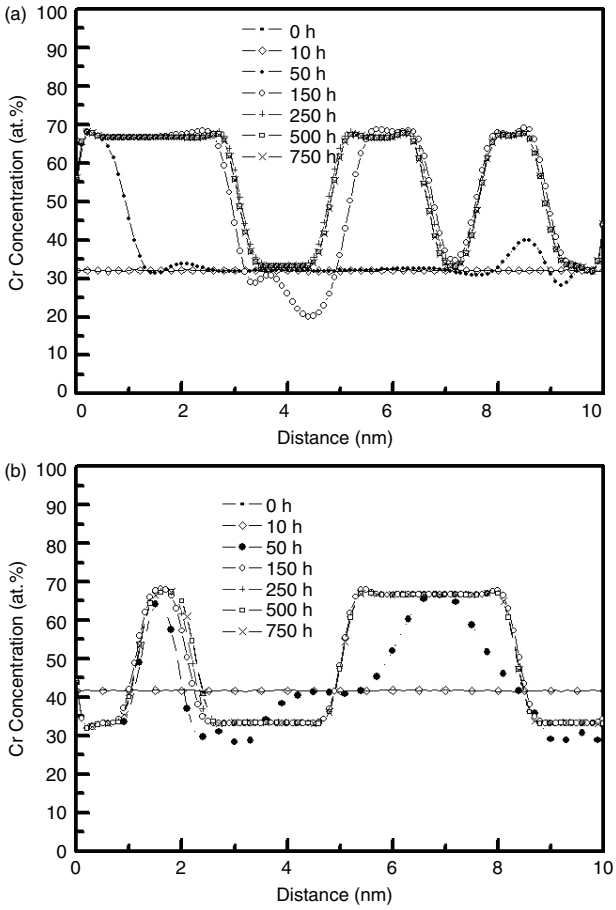

FIGURE 2. Concentration profiles of the: (a) Fe-32 and (b) 40 at.% Cr alloys aged at 470 °C for different times using the linear equation.

In contrast, Fig. 2 (a and b) show the concentration profiles for both alloy compositions after aging at 470 °C for different times obtained by the linear equation. The increase in the amplitude of composition modulation is also observed with the increase in time for both the aged alloys. This fact confirms the presence of the spinodal decomposition mechanism. Nevertheless, the increase in modulation amplitude is lower than that corresponding to the nonlinear equation, Fig. 1. This behavior can be explained considering the value variation of $\frac{\partial^2 f}{\partial c^2}$ within the miscibility gap. This term appears in the linear equation, Eq. (2), and it is negative for an alloy composition which is located within the chemical spinodal of the equilibrium phase diagram and it becomes positive for a composition outside of it. Thus, the modulation amplitude can only growth if this second derivative is less than zero and therefore the amplification factor $R(\lambda)$ is greater than zero according to the Cahn-Hilliard theory of spinodal decomposition (Cahn and Hilliard, 1971). Then, if the decomposed phases have compositions located outside of the chemical spinodal, the composition modulation cannot continue increasing its amplitude as the aging progresses because the second derivative of free energy is positive. On the other hand, the second derivative is not present directly in the nonlinear equation, Eq. (1). Consequently, the amplitude of composition modulation growths continuously meanwhile the equilibrium composition value of the decomposed phases (miscibility gap of the equilibrium phase diagram) is not reached, as observed in Fig. 1. The concentration profiles obtained at 500 °C using both equations showed faster growth kinetics of the composition modulation because of the fast atomic diffusivity (Mehrer, 1990).

4.2. Morphology of the decomposed phases

Figures 3 and 4 show for instance the simulated microstructural evolution, based on the Cr concentration, of the phase decomposition in the Fe-40-at.% Cr alloy aged at 470 °C for times from 10 to 750 h using the nonlinear and linear equations, respectively. The white and gray zones

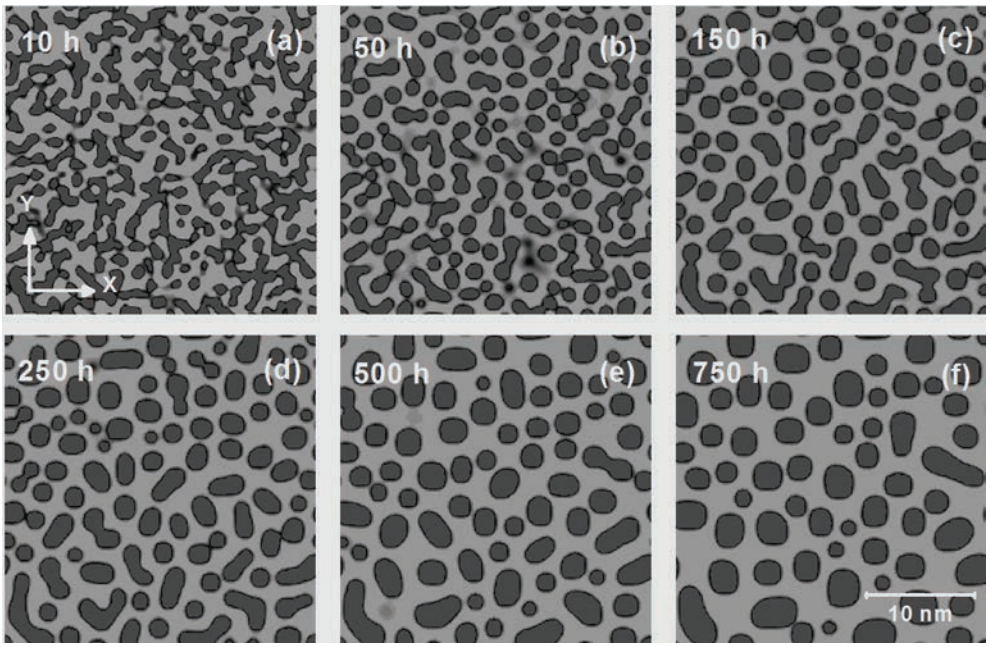

FIGURE 3. Simulated microstructural evolution based on the Cr concentration of the phase decomposition of the Fe-40 at.% Cr alloy aged at 470 °C for: (a) 10, (b) 50, (c) 150, (d) 250, (e) 500 and (f) 750 h using the nonlinear equation.

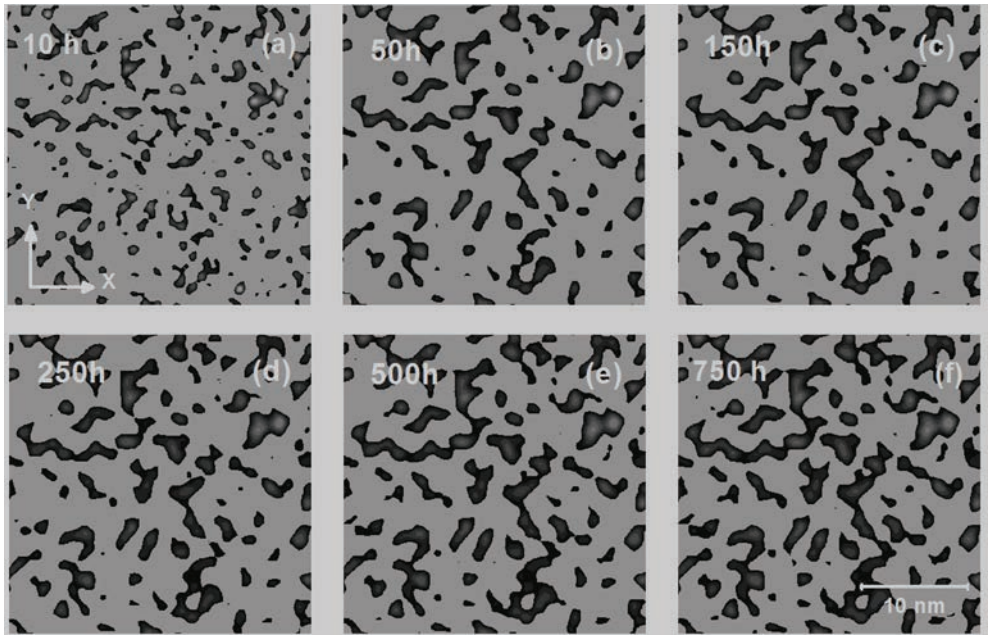

FIGURE 4. Simulated microstructural evolution based on the Cr concentration of the phase decomposition of the Fe-40 at.% Cr alloy aged at 470 °C for: (a) 10, (b) 50, (c) 150, (d) 250, (e) 500 and (f) 750 h using the linear equation.

represent to the Fe-rich and Cr-rich phases, respectively. It can be observed and irregular and interconnected morphology of the decomposed phases in the alloy aged for times up to 10 h for both equations, Figs. 3 and 4a. This morphology characteristic is known as percolated structure and it has been commonly observed to occur during the early stages of aging in the spinodally decomposed alloys (Cahn and Hilliard, 1971). Nevertheless, the degree of interconnection is much lower for the linear equation because of the lower volume fraction of the Cr-rich phase. In the case of the simulated

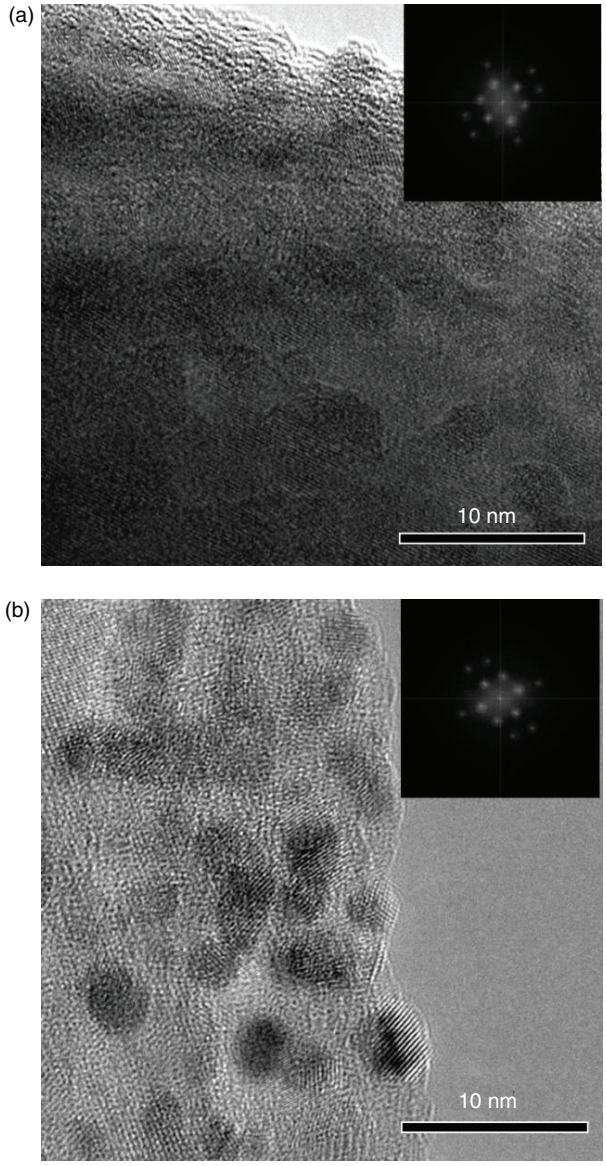

FIGURE 5. HR-TEM micrographs of the Fe-40 at.% Cr alloy aged at 470 °C for (a) 50 and (b) 500 h.

microstructure at 50 h, the percolated microstructure is still observed in the decomposed alloy for the linear equation, Fig. 4b, while a clear separation of the decomposed phases can be observed for the nonlinear equation, Fig. 3b. Furthermore, the morphology of Cr-rich phase is close to spheres. The HR-TEM micrographs of the Fe-40at.% Cr alloys are shown in Fig. 5 (a and b) after solution treating, quenching and aging at 470 °C for 50 and 500 h. Figure 5a shows that the decomposed phase are irregular and interconnected, similar to the simulated microstructure for the same alloy at 10 h using both linear and nonlinear equations. In contrast, the HR-TEM of this alloy at 500 h shows clearly the presence of spheres corresponding to

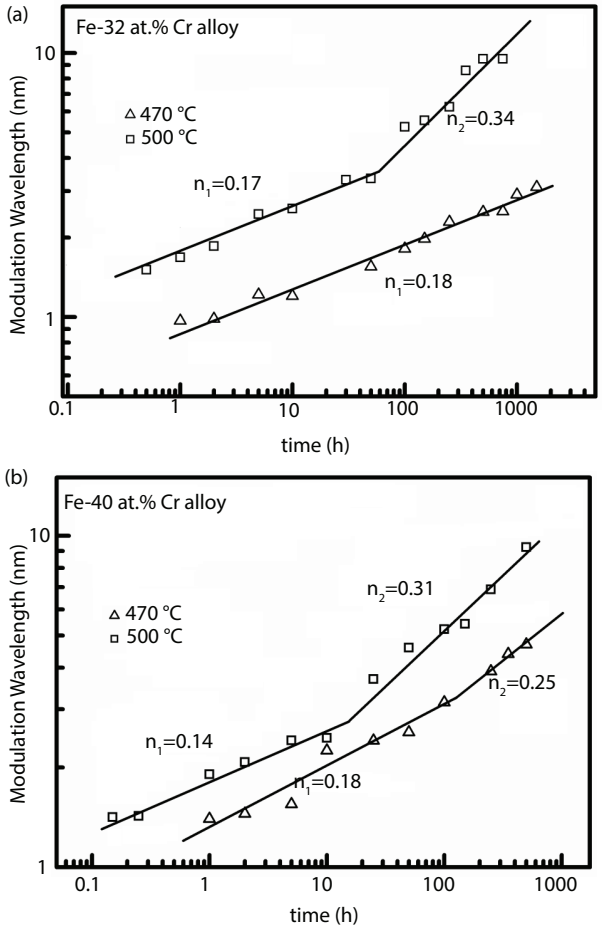

FIGURE 6. Plot of modulation wavelength l versus aging time t for the: (a) Fe-32 at.% Cr and (b) Fe-40 at.% C alloys.

the Cr-rich phases embedded in the ferrite phase matrix, Fig. 5b. The decomposed phases present a coherent interface. This shape of decomposed Cr-rich phase is in good agreement with the simulated microstructure, Fig. 3 (e and f), using the nonlinear equation. The simulated microstructure of linear equation still shows a percolated structure which corresponds to the early stages of aging. This above morphological characteristics suggests that the linear Cahn-Hilliard equation is more suitable to describe the spinodal decomposition at the early stages as suggested in the spinodal decomposition theory (Cahn and Hilliard, 1971). The nonlinear equation seems to be appropriate to describe the evolution of decomposed phases at both the early stage and the coarsening stage.

5. DISCUSSION

The variation of the wavelength λ of composition modulation as a function of time is shown in Fig. 6 (a and b) for the Fe-32 and 40 at.% Cr alloys, respectively, aged at 470 and 500 °C for different times.

The modulation wavelength was determined using the correlation analysis (Hyde *et al.*, 1995) of the concentration profiles shown in Fig. 1. This analysis has been used to determine the inter-particle distance in AP-FIM concentration profiles.

The kinetics growth rate for the wavelength variation with time can be analyzed using the following equation:

$$\lambda = k\, t^{n} \qquad (11)$$

where k is a rate constant and **n** is the time exponent. The time exponent n_1 corresponds to the early stages of aging, while the exponent n_2 is related to longer aging times. These were determined to be about 0.14–0.18 and 0.0.25–0.30, respectively, for the aging at 470 and 500 °C. The slow growth kinetics noticed at the early stages has been related to the spinodal decomposition because a coarsening process of clusters is expected to follow a time exponent close to 0.1 (Kostorz, 2001, Soriano *et al.*, 2010). A time exponent of about 0.2 was determined for the concentration evolution in the Fe-45wt.% Cr alloy aged at 500 °C by PoSAP technique (Hyde *et al.*, 1995). This value is in good agreement with that of present work. On the other hand, the fast growth kinetics for prolonged aging time can be associated with the coarsening stage of the decomposed phases because a time exponent of about 0.333 is predicted for the diffusion-controlled coarsening (Cahn, 1966, Voorhees, 1992, Kostorz, 2001, Soriano *et al.*, 2009). A value of modulation wavelength was determined to be of about 4 nm by FIM in the Fe-32 at.% Cr alloy aged 470 °C for 50 h (Brenner *et al.*, 1982). It is also interesting to notice that the growth kinetics of spinodal decomposition is faster in the aged Fe-40at.% Cr alloy and thus the coarsening stage starts earlier than for the other alloy composition. This behavior can be attributed, as explained above, to the higher driving force for the spinodal decomposition in this composition.

6. CONCLUSIONS

The analysis of spinodal decomposition in Fe-Cr alloys using the nonlinear and linear Cahn-Hilliard equations shows that both equations reproduces the main characteristics of spinodal decomposition expected in the aged Fe-Cr alloys according to the spinodal decomposition theory. Nevertheless, the morphology of decomposed phases for simulation with linear equation is more representative of the phase decomposition at the early stages of aging. In contrast, the nonlinear equation reproduces both the early and later stages of aging in the aged Fe-Cr alloys.

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