Modeling of thermodynamic properties of (Fe-Ni-C, Fe-Cr-C) alloys using computational approach

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Abstract

The paper shows the thermodynamic properties of alloys Fe-Cr-C, Fe-Ni-C system using modeling and simulation approach. The thermo-calc software with databases is utilized for calculations and results. The calculation shows alloying at (1900K-2000K) temperature range. The atmospheric pressure is kept constant 10^6 Pascal. The active phase at 1900K is liquid phase with ≈ 0.5 mass % for C compositions. The total Gibbs energy is found decreasing in the Fe-Ni-C system, which shows the stability of the system. The solubility of Cr is found less than the solubility of Ni in the Fe-C system as investigated during activities simulations. The enthalpies of formation of the system are found of the near linear relation with temperature raise and coupling properties of the alloying. BCC phase of enthalpies formation is more responsive then BCC of enthalpy during alloying. The Fe-Ni-C shows negative deviations from Raoults law and corresponding positive deviations from Vegard's and Henry law. The withstanding phase is graphite with highest thermal expansion coefficient. The highest T-zero fluctuations is noted in the Fe-Cr-C system. The alloy shows the less solubility of the carbon at low temperature, while results the great alloying at higher temperature in the Fe-Ni-C system better industrial aspects.

Keywords: Calphad method, fe-demo databases, high entropy system, mechanical study, thermodynamic calculations,

1. Introduction

The Fe-rich region is reassessed on the basis of transition temperature and studied the boundary of phases in the Fe-Ni-C ternary alloy system. The phase diagram of Fe-Ni alloy are get together with experimental results and found in agreements at 20 degree temperature for the Ni reach side. (I.E. Tsypin. (1983), A. A. Zhukov *et al.,* (1984).The optimization are carried out by the researchers to evaluate the Gibbs energy of the ternary alloys Fe-Cr-C for computing the stability of phases (D.A. Mirzaev *et al.,* (1988).The data obtained for the calculation of thermodynamic properties of the Fe-Ni-C ternary alloy system were found higher values then the already calculated results in Fe-Cr-C system during optimization (AN. Emelyushin. (2016).The researchers optimized the Fe-Ni-C ternary system by the help of crystallization elution fractionation (CEF) analytical techniques for solid solution phase's investigations. They found many phases in the phase diagram of the

given alloy system as liquid, FCC (face centered cubic), BCC (base centered cubic) and cementite phases (F. Maratray *et al.,* (1970).The strongest deviation from Raoults law in negative side is observed by the researchers between Ni and Fe atoms, and studied on the basis of MQM (modified Quasichemical model) methods and interpolation methods (K.yu. Okishevb. (2011). the present work is performed to discuss all the parameters of the Fe-Cr-C, Fe-Ni-C ternary alloys system to evaluate the thermodynamic properties to perform predictions for the better alloying of the system. The Anderson and lee used the TC window for calculations of alloys, which is the basic for the current research work. The initial opted calculations taken for Gibbs free energy are rescued from Dinsdale calculations (J.-O.Andersson *et al.,* (2002). The Fe-Ni-C system was thermodynamically analyzed by MQM model (modified Quasichemical model).The pairs approximations are used for the asymmetry alloying and studied the solubility of Ni rich sections. The solubility of the carbon is found minimum at the ordering of Fe-Ni-C system during Ni-rich phase (Min-Kyu peak *et al.,* (2021). The alloys with greater Ni concentrations are important for mechanical properties sectors. The highest Ni contents improve the steel designing applications of the alloy Fe-C-Ni. The differential scanning calorimetric procedure was utilized for Ni of 30wt% and studied the wide range of enthalpy mixing operations of alloying. The carbon range solubility in the Fe-Ni, Fe-Cr alloy is studied at 1500^0C and 1600^0C and calculations were assessed by Factsage software and MQM methods (A.D. Pelton, (2000)., K. Shubhank & Y.B. Kang. (2014)., A.T. Dinsdale. (1991).

2. Procedure

The Gibbs free energy of the Fe-Ni-C system were studied by the use of compound energy model and stable phases modeled for the prediction of the phase equilibria of the Fe-Ni-C ternary alloy system (C.W. Bale, E. Be ´lisle, *et al.,* (2016)., Waseem Ullah shah *et al.,* (2022). The computational approaches play a vital role in the field of materials science and engineering. The material properties and phase equilibria for materials design is the basic operations of computational analysis. The Calphad method is the basic computational method for thermodynamic investigations of the alloy system and calculations of thermodynamic properties. Hydrothermal method of materials synthesis is now day's remarkable method for materials specifications. The grain size diameters and crystalline sizes can be increases with annealing (Nada Falih M *et al.,* (2021)., Sumaryada *et al.,* (2019)., Senkov, O.N *et al.,* (2015). All the calculations in the research paper are performed by the Calphad method based on the thermo-calc software, the FeDemo databases are used for calculations and simulations. The calculation are executed by correlations cumulant expansion theorem as,

$$G_m^{liquid} = (x_1 + 2x_{1,2} + x_{1,2}) \circ G_1^{liquid} + (x_2 + x_{1,2} + 2x_{1,2}) \circ G_2^{liquid}, \quad \text{while,} \tag{1}$$

While G_m^{liquid} shows the total magnetic part of Gibbs free energy of alloying system. $x_{1,2}$ Shows the composition of alloying elements.

$$+x_{1,2}\Delta G_{1,2}^{liquid} + \mathrm{RT}\,(x_1 \mathrm{Ln} x_1 + x_{1,2} ln x_{1,2} + x_2 \ln x_2)\, x_1 x_{1,2} {}^{\circ}L_{1,2}^{liquid} \quad \text{while,} \tag{2}$$

$L_{1,2}^{liquid}$ Indicates the coupling orbital moment of alloying elements as per the cumulant correlation expansion theorem procedure.

$+x_1x_{1,2}{}^{o}L_{1,2}^{liquid}+x_1x_2{}^{o}L_{1,2}^{liquid}+x_{1,2}x_{1,2}{}^{o}L_{2,2}^{liquid}+x_2x_1{}^{o}L_{2,1}^{liquid}$ while, (3)

$o_g^{m\Phi}$ Seem the orbital moment of the alloy with Φ as a coupling factor. ${}^{o}G_2^{liquid}$ shows the magnetic part of Gibbs free energy for the adding element

$o_g^{m\Phi} = \sum_i^n = 1{,}2\, x_{1,2}{}^{o}G_{1,2}^{\Phi} + \mathrm{RT} \sum_i^n = 1{,}2\, x_{1,2}\ln x_{1,2} + {}^{xs}G_m^{\Phi}$, Φ as , (4)

Δ $G_{1,2}^{liquid}$ shows the change in magnetic moment of alloying element during phase transition. $\mathrm{Ln}x_{1,2}$ represents the angular symmetry of alloying elements. ${}^{o}G_{1,2}^{\Phi}$ is for molar Gibbs free energy of alloying elements. ${}^{xs}G_m^{\Phi}$ is the interaction Gibbs energy of alloy formation. RT shows the product of ideal gas constant and temperature, which describe here the internal energy to the system (S Sheibani, S Heshmati-manesh *et al.,* (2010). The mechanical properties like crack susceptibility coefficient, Yielding strength and Precipitation simulations from cementite to ferrite of the Fe-Cr-C/Fe-Ni-C are investigated and the results are predicted on the basis of Calphad method operations (Waseem Ullah Shah *et al.,* (2022).Thermo-mechanical calculations of Fe-Ni-C alloys are carried through Calphad method, coercive energy analysis, interfacial energy analysis, density analysis, molar volume evaluations and apparent heat capacity of the Fe-Ni-C are plotted. (Waseem Ullah Shah *et al.,* (2022).

3. Briefly highlights of software package specifications

The specification of the TC-window is given; it is the compatible and most approachable package in the field of materials sciences and engineering. The specification is explored on the basis of the system requirements and software modules for simulations. The execution codes and Terminologies are enclosed into the window of the package for evaluation and assessment of your results. 50 GB of free disk space needed with SSD solid state disk, 16GB of RAM, TAB modules for mixtures and chemical reactions. Thermo-calc 2022a versions need SSSE3 instruction CPU with Windows 64-bit, 10, 11. Diffusion module. DICTRA, Precipitation module, TC-PRISMA, TC-Python and PARROT modules are used for evaluation, assessment of the data (J-O Anderson, Thomas Helander *et al.,* (2002).

The results are compared with recent finding of literature. The research work performed in the MS is the afresh attempt for the simulations of the Fe-Cr-C/Fe-Ni-C alloys. The properties calculated through database calculations are plotted with thermodynamic descriptions. The enthalpy formation and Gibbs free energy modeling is manipulated for the thermodynamic parameters varying techniques to get the literature verified. The high entropy alloy natures of the alloys are verified by generating entropy of formation procedure for the system. The systems are valid and most research oriented field in the high entropy sector. The table 1 shows the literature work performed on the research assessment of the Fe-Ni, Fe-Cr alloys doped with C compositions.

Table 1. Work of literature for thermodynamic properties. Alloys, Fe-Cr, Fe-Ni, Fe-Cr-C, and Fe-Ni-C at different elevated temperature ranges.

Liquidus temperature for seven Fe-Cr alloys using thermal pyrometers.	W. Xiong *et al.,* .2010
High-temperature phase equilibria in the Fe-Cr system were contributed.	W. Xiong *et al.*,2010
enthalpy of mixing of the BCC phase in the paramagnetic state. Fe (0.6) wt %, 1185-1667K Comparison of the activity at1173K.	W.B. Kendall, *et al.,* 1973,J.O. Anderson *et al.,* 1987
Ab-initio calculations of Fe-Ni system describe Fe 0-0.5 with (0-5) KJ/mol enthalpy increase ,1600K.	korzhavyi et al.2009, Olsson *et al*.2006
Isothermal section investigations for Fe-Cr-C at 1773K with carbide phases, Cr_3C_2, Cr_7C_3, $Cr_{23}C_6$ Graphite on top stable scale. 0.4-0.6 mole fraction Cr	Luoma *et al.,* 2002
Calculation of isothermal section in Fe-Cr alloys for Fe, Cr (0.05) mass percent at 1273K,	Alexandra. Khvan *et al.,* Calphad 2014
Investigations of Coercive energy analysis, interfacial energy analysis, interfacial energy calculations at 1900K for Fe-Ni-C_X $_{(X=0.4)}$ system.	Waseem Ullah Shah *et al* ,2022
Positive deviation from ideality at $_{0.7}$Fe, $_{0.5}$Cr of the activities at 1173 K between experimental data and calculated results from CALPHAD modeling.	W. Xiong *et al.*2010
Used Calphad simulations by using highest temperature of 2175K. Total Gibbs energy found (-119043) J/mol.	S.M. Shah *et al.,* 2018
Shown the thermodynamic properties of alloys Fe-Cr-C, Fe-Ni-C system using modeling and simulation approach. BCC of entropy is more responsive then BCC of enthalpy during alloying. The Fe-Ni-C shows negative deviations from Raoults law and corresponding positive deviations from Vegard's and Henry law.	This work

4. Results and discussion

The section shows all the modeling and simulations carried by TC window for getting the results. The results are crass verified by predicting the precise matrix. The alloying matrixes are feasible for Ni and Cr rich matrix for proper doping and mixings.

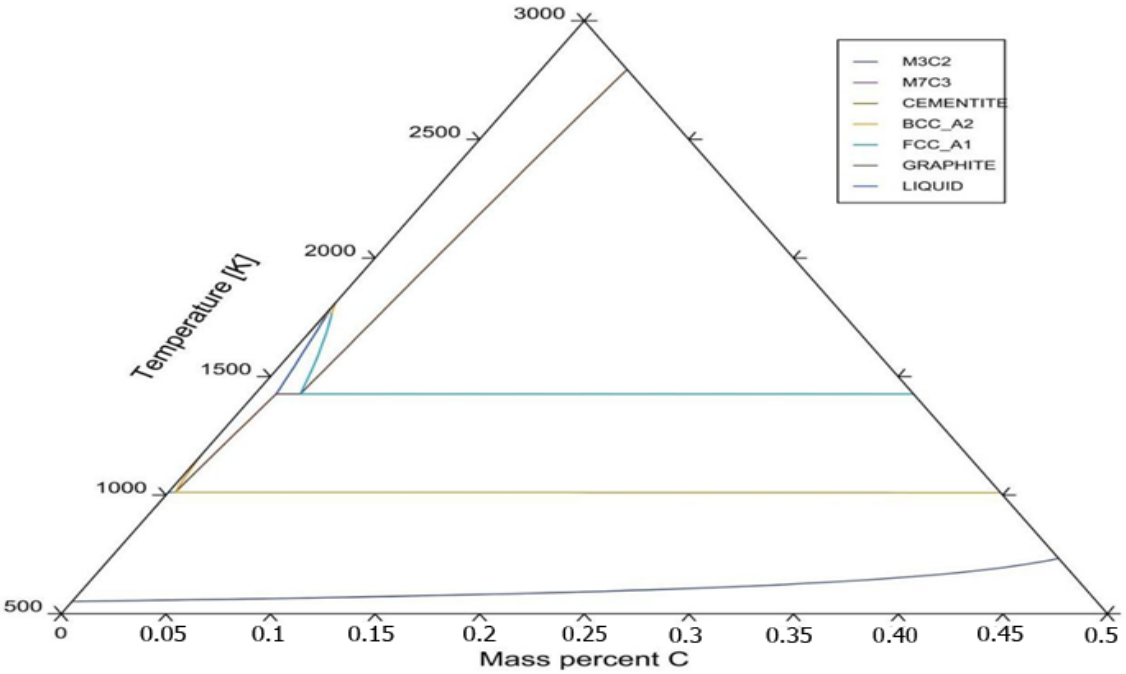

Fig. 1. Phase analysis, annealed at 1900K. BCC phase is found with highest spread and Cr-rich section

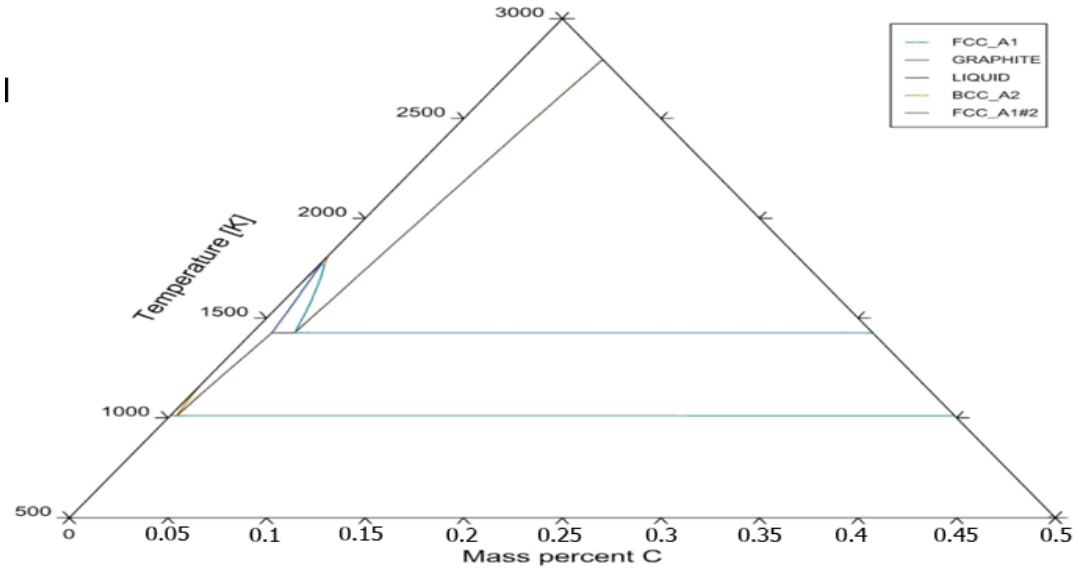

Fig. 2. Phase analysis section of the Ni rich solubility in the Fe-C system. Graphite phase is found highest molar volume in Ni-rich section for better solubility of Ni.

Phase diagrams for phase analysis of Fe-Cr-C, Fe-Ni-C alloys are assessed. The mass percent of Cr found is 14.44 and C of 0.5 mass percent with enthalpy 52000.3 J/K. The total Gibbs energy of the system Fe-Cr-C is found -11000.089J/mol. The active phase at 1900K is liquid phase with 0.36381 mass percent of Cr, and 0.5 for C compositions. The final withstanding phase is graphite with the thermal expansion coefficient of 0.85021 um/m.K. The Fe-Ni-C phase profile is assessed with modeling and simulations process .For the most active phase, the enthalpy is found 35000 J/K with total Gibbs energy of -14000 J/mol. The temperature is maintained 1900K with changing the mass percent of carbon and nickel as 0.5, 0.1 of numerical value. The thermodynamic potential of -41.62 for Kelvin increases, which results the maximum bonding of alloying elements. The active phase at this composition is liquid with the expansion coefficient of 0.152 um/m.K while the mass and mole fraction of the Fe is noted 0.53669, for C is 0.016579 of composition. The last active phase withstand is graphite with the given profile as 0.84 um/m.K of thermal expansion coefficient, while the carbon is 1.00 mass percent composition with 0.00 composition of Ni and Fe. The final withstanding phase is Graphite with the thermal expansion coefficient of 0.85021 um/m.K for 0.5 C. The activity of the carbon is found maximum 0.07016 while less for Ni and Fe as 0.00018, 0.00023.The active phase at this composition is liquid with the expansion coefficient of 0.15235 um/m.K, the mass and mole fraction of the Fe is noted 0.53669, 0.60642, for Ni 0.29752, 0.35329, for C is 0.016579, 0.04029 of composition in Fe-Ni-C system. The alloy shows mechanical flexibilities and better doping.

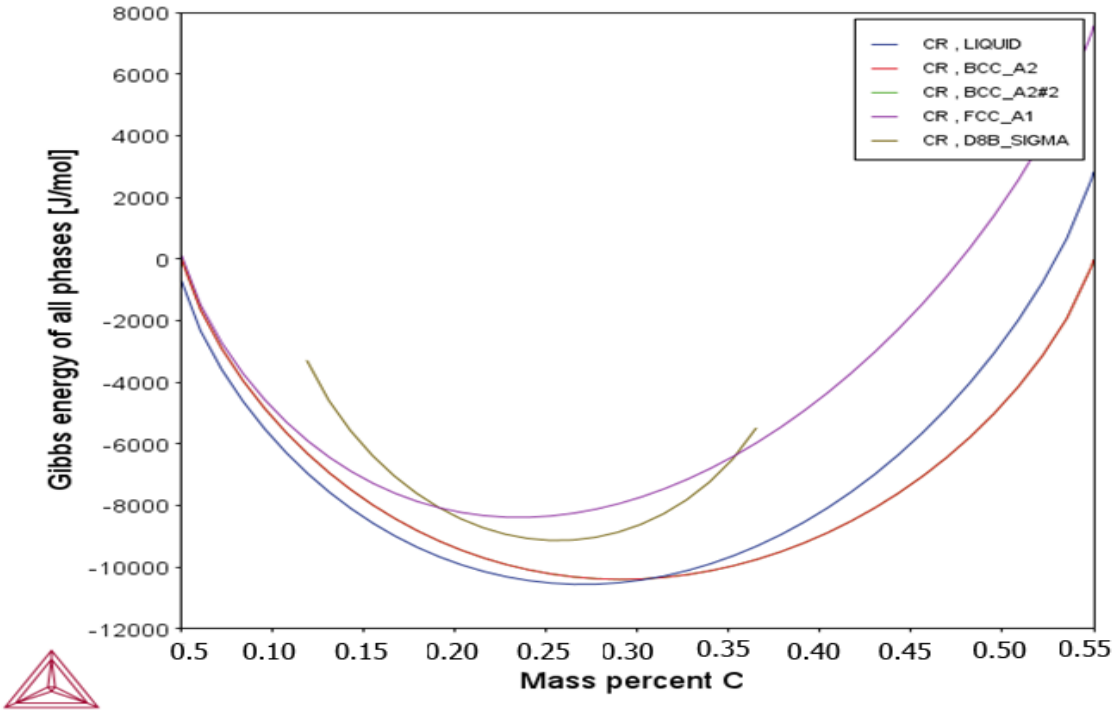

Fig. 3. Gibbs free energy of region Cr doped. The less Gibb energy value at 1900K shows Less Solubility of Cr-rich section.

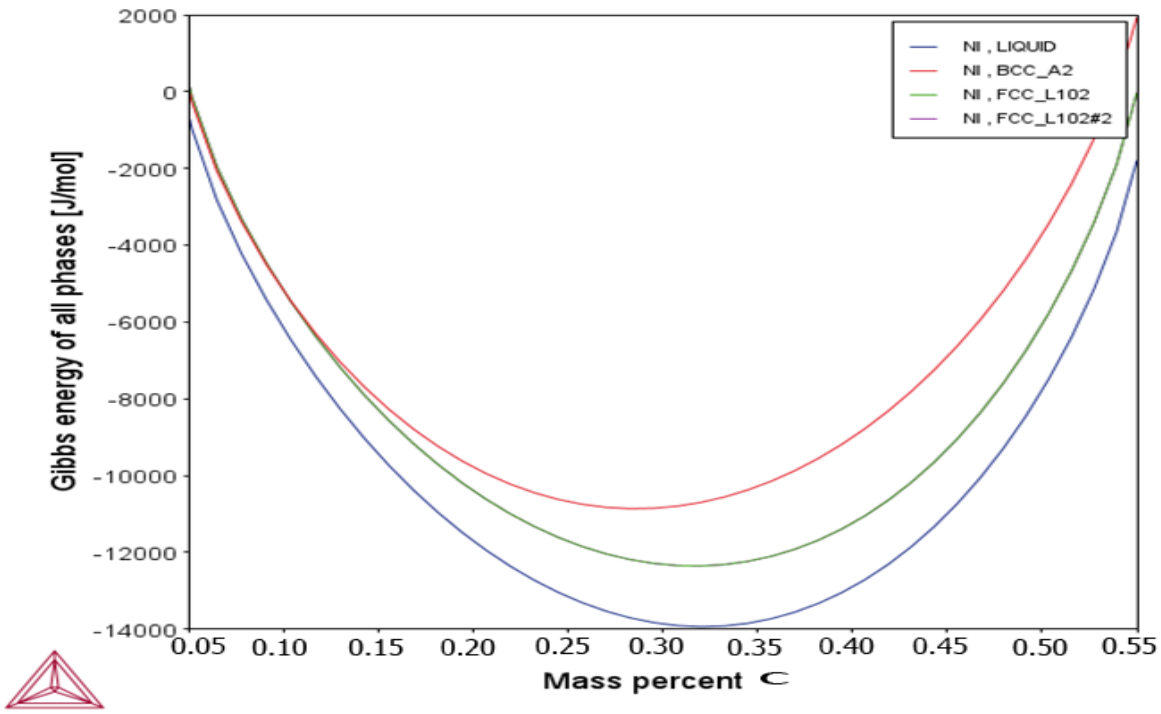

Fig. 4. Gibbs free energy of the region Ni doped with highest solubility in Fe-C system.

The modeling is based on the addition of Cr; Ni in the Fe-C based system. The Gibbs free energy of the Ni-doped alloy is showing more decrease and results more stability of the system. The sigma phase in the Cr-doped alloy system shows critical area Gibbs free energy and results rare doping characteristics in the system. For the Cr-doped Gibbs energy cure, the maximum Gibbs free energy is seen for BCC_A_2 at 0.20-0.35 mass % of C composition in alloying. The FCC is showing less Gibbs energy after 0.20-0.30 mass% of C contents in alloying. The maximum spread of Gibbs energy for the sigma phase is found for 0.15-0.38 mass% of C adding in the alloy. For the case of nickel as adding elements, the FCC is having more Gibbs free energy and contributes more better alloying for 0.25-0.40 mass% of Ni-doped region. The rare Gibbs energy is noted for BCC with 0.27-0.35 mass % of Ni-doped contents during alloying. The chromium contents with rare solubility during alloying results less total Gibbs energy and the Ni-doped FCC results better total Gibbs energy in the system. The maximum decrease in the Gibbs free energy of the Ni-doped region describes the more hardness and mechanical stability of the FCC doped regime. The more toughness and yielding are the results of the given alloy as a result of Ni addition. The chromium with rare solubility in the Fe-based alloys contributes less hardness and toughness of the alloy system.

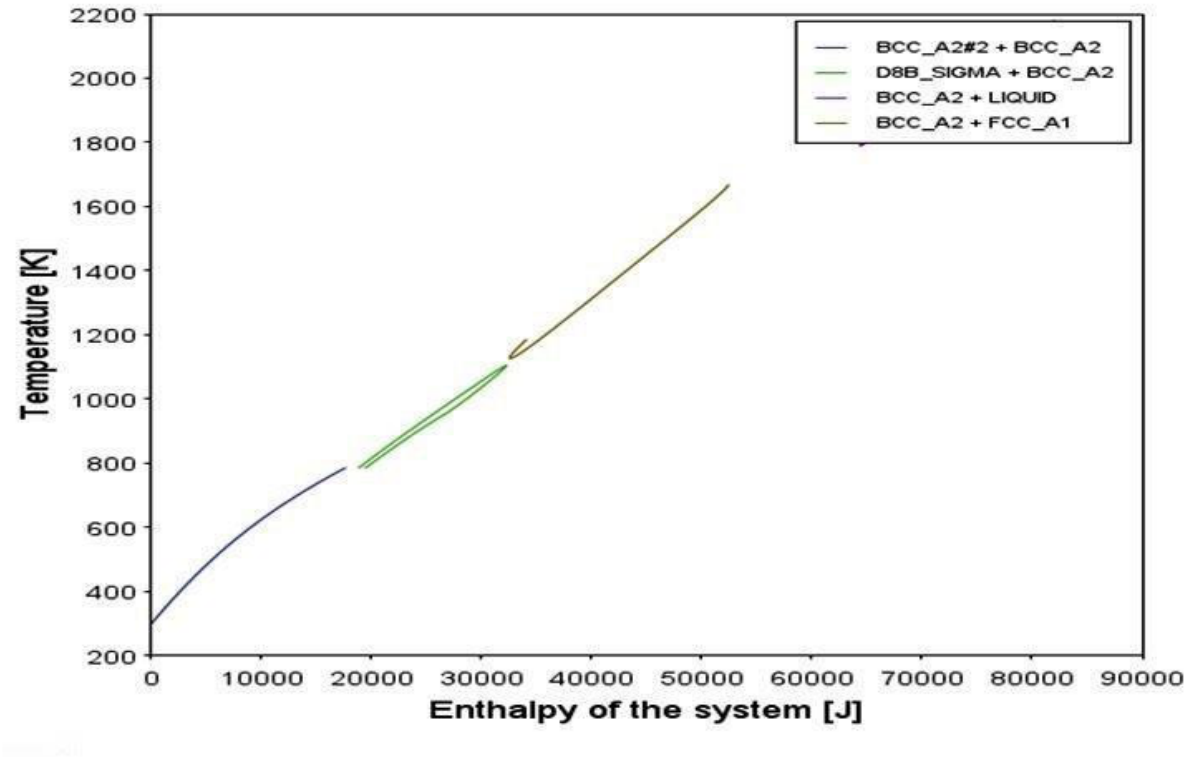

Fig. 5. Enthalpy formation of the region Cr doped at annealing of 1900K.

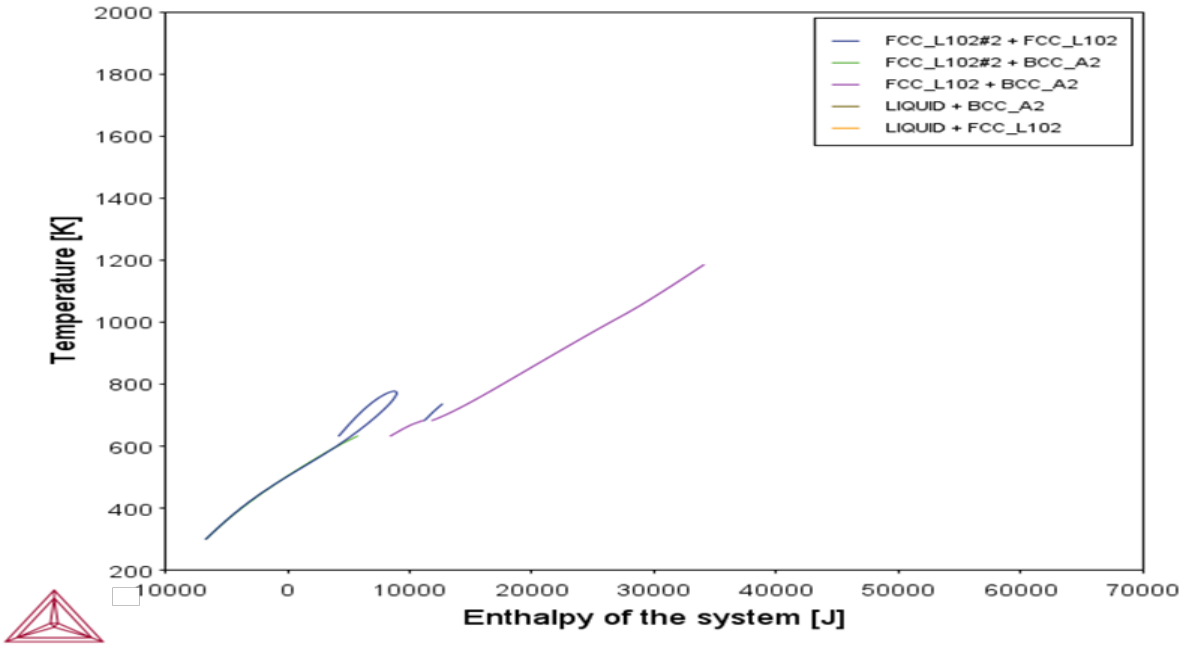

Fig. 6. Enthalpy of the region Ni doped at annealing of 1900K. Ni-rich section increases the entropy of BCC Phase of alloying at that Coupled Region shows still stability.

The enthalpy responds to the temperature feasible as found during simulations. The BCC_A_2 of the enthalpy covers alloying for the 300-800K during annealing process. The sigma phase with less activity in alloying is found for the 680-1100K of annealing temperature. The BCC is found active phase in enthalpy formation during 1300-1700K. The enthalpy of the system increases gradually with temperature verses .The enthalpy results the more heating contents of the system of alloying. Entropy of the system is found more responsive to the temperature increased during alloying. During 0.20-0.35 mass% of alloying composition and 300-800K of annealing temperature results BCC_A_2 phase arising activity. The sigma phase is found during 32000 J of enthalpy of alloying at temperature range of 700-1100K. BCC_A2 and FCC coupled regions are found 54000 J of enthalpy alloying at the temperature range of 1200-1700K. The entropy of BCC_A_2 is found maximum and more responsive with linear accordance with temperature. The more entropy of the system indicated the more activity of the alloying system with rare equilibrium for the given phase. The alloy with Ni-doping found more responsive and feasible for alloying.

Table 2. Thermodynamic database calculations at elevated temperature for Cr rich section.

Mass %Cr	Mass % C	Moles	Mass :G	T: k°	Total Gibbs Energy: J/Mol	Enthalpy :J/K	Volume:M³	Mole Fraction	Mass Fraction	Potential	Activity
14.44707	0.5	1.0	15.21183	1900	-11000.08959	52000.3	5.77240E-6	0.92327 :C	0.72900: C	-41974.62608	0.07016 :C
	--		--	--	-11000.08959	52000.3	--	0.04227 :Cr	0.14447: Cr	-1.41575E5	0.00013: Cr
	--		--	--	-11000.08959	52000.3	--	0.03447 :Fe	0.12653: Fe	-1.37976E5	0.00016:Fe
LIQUID #1		0.11617	4.59621	--	-11000.08959	52000.3	0.14979 fraction	0.36381 :Cr	0.47815 :Cr	--	--
	--		--	--	--..	52000.3	--	0.29667 :Fe	0.41878 :Fe	--	--
			--	--	--	52000.3	--	0.33952 :C	0.10307 :C	--	--
GRAPHITE#1	--	0.88383	10.61563	--	--	--	0.85021 fraction	1.00000 :C	1.00000	--	--
	--	--	--	--	--	--	--	0.00000 :Fe	0.00000	--	--
	--	--	--	--	--	--	--	0.00000 :Cr	0.00000	--	--

For the Fe-Cr-C system, Graphite Phase is more stable indicating highest Cr solubility and perfect Alloying at 1900K atmospheric pressure is kept constant 10^6 Pascal. The graphite phase are sorted the most stable alloying phase with maximum temperature maintenance. The enthalpy of the system increases up to 52000 J with constant interface .The Gibbs energy of the Fe-Cr-C system acquires the lowest value of -10000.08959 J/mol. The decrease in the Gibbs energy value shows negative deviation of the alloy system and better stability at highest temperature 1900K.the Activity values in the given table 2 increases result increases the enthalpy value and heat contents

of the system. The potential of molecular bonding increases further, which shows the stable bonding and epitaxial growth of the alloying elements Fe, Cr, C .the alloying shows the epitaxial growth for the lowest activity in the Fe-Cr-C system. The higher activity of the Fe-Ni-C alloy system shows the highest growth of the Ni composition in the system. The enthalpies of the both alloys are high, which result the highest heat contents and the heat mode of the alloy. The entropy of the both alloys is smoother for alloying. The Ni composition with highest solubility in the Fe-C system results more entropy of the given ternary system.

Table 3. Thermodynamic database calculation of Ni doped matrix at elevated temperature.

Mass %Ni	Mass % C	Moles	Mass :G	T: k°	Total Gibbs Energy: J/Mol	Enthalpy :J/K	Volume:M³	Mole Fraction	Mass Fraction	Potential	Activity
0.1	0.5	1.0	16.66899	1900	-14000	35000	5.79824E-6	0.89672: C	0.64614: C	-41974.62608:C	0.07016: C
	--		--	--	-14000	35000	--	0.04601: Ni	0.16198: Ni	-1.32877E5 :Ni	0.00022: Ni
	--		--	--	-14000	35000	--	0.05727: Fe	0.19188: Fe	-1.34878E5:Fe	0.00020:Fe
LIQUID #1		0.12185	6.12150	--			0.15901 Fraction	0.47002 :Fe	0.52249 :Fe	--	--
	--		--	--			--	0.37756 :Ni	0.44107 :Ni	--	--
			--	--			--	0.15242 :C	0.03644 :C	--	--
GRAPHITE#1	--	0.87815	10.54749	--			0.84099 Fraction	1.00000: C	1.00000: C	--	--
	--	--	--	--			--	0.00000: Fe	0.00000: Fe	--	--
	--	--	--	--			--	0.00000: Ni	0.00000: Ni	--	--

For the Fe-Ni-C system, The Result shows maximum solubility and alloying of Ni-rich Section in the Fe-C system at 1900K. Atmospheric pressure is kept Constant 10^6 Pascal for epitaxial growth of alloying. The graphite phase is the most retained phase in the Ni-C adopted alloys of Fe. The activity values of the Ni solubility increases and results the smooth alloying as compared to the addition of Cr in the given alloys system. The Fe composition is maintained higher as a base, while the activities of the Cr, Ni, and C are executed inside the alloy with 0.3-0.5 mass% of composition. The table 3 shows the thermodynamic calculations and modeling of the Fe-Ni-C ternary alloy system. The graphite is sorted the most temperature withstanding interface. The maximum thermodynamic molar activity of carbon is found 1 mol during alloying. The enthalpy is found temperature proportional and acquire a value of 35000.91973 J. the total Gibbs energy of the Fe-Ni-C system acquires a value of –14000.22892 J/mol. The maximum decrease in the Gibbs energy conversely to enthalpy shows the stability of the given alloy system. The potential of the Ni added Fe-Ni-C system is more the Cr added system, and the growth properties enhances better fraction in the Fe-Ni-C ternary system. The rare solubility of Cr in the Fe-C system is shown by activity calculations and chemical potential.

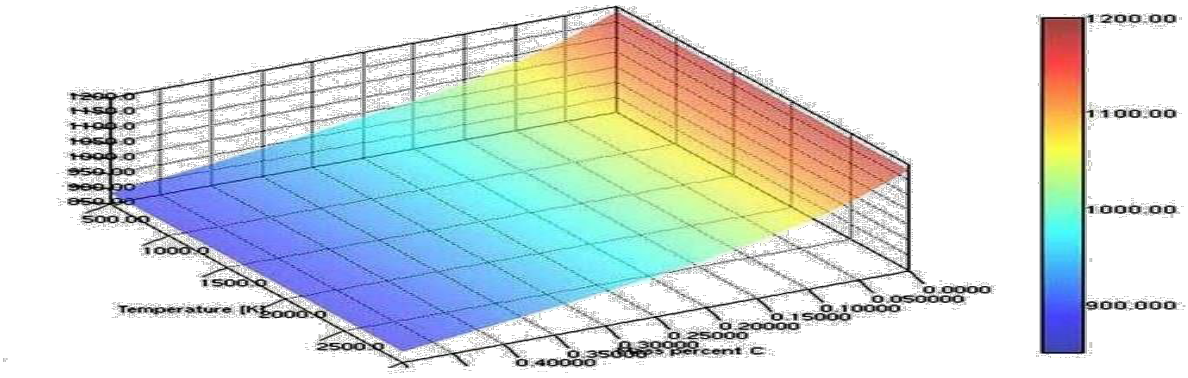

Fig. 7. T-zero analysis profile of Ni doped region at elevated temperature ranges.

The T-zero profile for the Fe-Ni-C ternary alloy system is given. The maximum T-zero is seen 1100.22907 values with temperature period of 1090-1200K.the alloy composition are 0.00-0.05 for carbon at highest ranges is seen. The Ni and Fe is noted 0.01, 99.99 of mass percent. The maximum carbon activity is noted as 0.4 mass percent with less temperature ranges of 500-750K.the alloy shows the less solubility of the carbon at low temperature, while results the great alloying at higher temperature. The doping and solubility of Ni-is found more than Cr addition, this results better alloying for BCC in Ni-doped regions.

Table 4. Energies simulations literature for given alloys.

The Gibbs free energy of the Ni-rich section of BCC is found more negative deviated from Raoults law.	J.O. Anderson *et al.,* (1987)
For Fe-Cr alloy, positive deviation is found from ideality with accurate accordance with Vegard's law.	S.M. Shah *et al.,* (2018)
Gibbs free energy is rescued for Fe-Cr system with stable configuration and parameters. Gibbs free energy, enthalpy, entropy for the upgraded ternary systems Fe-Cr-C /Fe-Ni-C at 1900K. **This Work**	Dinsdale *et al.,* (1991)

5. Conclusion

The paper predicted the thermodynamic based calculations, results based on simulations of the ternary alloys Fe-Cr-C, Fe-Ni-C system. The research work is performed by the applications of TC-window based on databases. The calculation shows modeling and simulations of the alloys at (1900K-2000K) temperature range. The atmospheric pressure is kept constant 10^6 Pascal. The total Gibbs energy of the system Fe-Cr-C is noted -11000 J/mol. The active phase at 1900K is liquid phase with 0.36381 mass percent of Cr, 0.29667 of Fe and 0.5 for C compositions. The final withstanding phase is graphite with the thermal expansion coefficient of 0.85021 um/m.K and the 1.00 for C. The activity of the carbon is found maximum 0.07016 while less for Ni and Fe as

0.00018, 0.00023. The active phase at this composition is liquid with the expansion coefficient of 0.15235.the lowest Gibbs free energy of Ni-doped region results the alloying stable. The alloy shows the less activity of carbon in the highest temperature in the Fe-Ni-C alloy system. The solubility of Ni-doped region is seen maximum during alloying, which results the epitaxial growth of alloying. The temperature is noted 500-3000K in the Fe-Cr-C system for better thermodynamic properties investigations. The least solubility of Cr-doped region BCC results non-epitaxial ordering of alloying. The maximum carbon activity is noted as ≈0.5 mass percent with less temperature ranges of 500-750K.The alloy shows the less solubility of the carbon at low temperature, while results the great alloying at higher temperature in the Fe-Ni-C system. For the Ni-doped region, the T-zero of 1100.22907 values with temperature period of 51090-1200K is observed. The enthalpy and entropy values seen fluctuation verses temperature. The enthalpy shows lower response with annealing process and shows better thermal parameters of the system. The entropy responses linear approximation verses temperature and shows the increase in the thermodynamic molar activity of the alloying. The results are important for metallurgical fields and thermodynamic phase analysis.

Conflict of interest

The authors do not have any possible conflicts of importance to declare.

ACKNOWLEDGMENTS.

This study was supported by Beijing University of science and technology Beijing, China for providing simulation and modeling tools of TC window.

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Submitted: 23/04/2022
Revised: 23/08/2022
Accepted: 24/08/2022
DOI : 10.48129/kjs.20257