Thermo-mechanical assessment of high entropy (Fe-Ni-$C_{x\ (X=0.3-0.5)}$), (Fe-Cr-$C_{x\ (X=0.3-0.5)}$ ternary alloys system using calphad method

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Abstract

The thermodynamical assessment of high entropy alloys (Fe-Ni-$C_{x\ (X=0.3-0.5)}$), (Fe-Cr-$C_{x\ (X=0.3-0.5)}$) system is performed in this research work through Fe-demo database and Thermo-Calc software package. The high energy thermal analysis is manipulated for yield strength from FCC to BCC, precipitation from cementite to M_7C_3 (grain boundaries), Crack Susceptibility Coefficient for Fe-Ni-C ,Fe-Cr-C ternary alloys system at (1900-3000)K temperature with constant atmospheric pressure of 10^6 Pascal. The highest crack susceptibility coefficient for Fe-Cr-C, Fe-Ni-C system is found 2.70, 2.60 with mass percent of C 0.11%, at 3000K of temperature with Mass percent. Yield strength from FCC to BCC is found 798 MPa, 36 MPa for Fe-Cr-C, Fe-Ni-C ternary alloys at the cost of 2.2, 0.1 mass% C. Phase transition is noted from cementite to M_7C_3 at 1346.77339 K. $FCC\_A_{1\#3}$ phases with 0.98772 moles and 0.01228 mole Of M_7C_3 with 0 moles of $M_{23}C_6$ carbide phases observed. The comprehensive line investigation of mechanical properties is justified with simulation/computational inputs. The results are feasible for industrial sectors and metallurgical centers for operation. The alloy shows equilibrium and good stability.

Keywords: Calphad method; Fe-demo databases; high entropy system; mechanical study; thermodynamic calculations.

1. Introduction

Iron based alloys are experimentally and theoretically investigated many times and showing main importance in steel industry and stainless steel tool factories. The carbide cementite phases are most common in steel and alloyed steel industries and have most extensive solid solubility as compare to other metals. Study reveals that Carbide of form Cr_3C_2 does not completely dissolve the iron constituents, which contributes less importance in designing steel alloys. Carbon phase stabilizes the austenite and ferrite phases as FCC and BCC, while the Cr stabilizes the ferrite BCC phase only. The BCC phase is remaining closer to the Fe-Cr Coupling, while the FCC phase expends upto appreciably extent and shows small solubility of carbon in the Fe-Cr system. As for the thermodynamic properties of Fe-Cr-C system, there is a vital lack of research analysis in

accurate data of high temperature in particular liquidus regions and around 973K. For the less temperature 973K, it is extensively needed further annealing to reach accurate equilibrium of the alloy system. The research background shows many uncertainties and contradiction for carbon solubility in ferrite phase BCC is still unknown for research areas. There is contradiction regarding the influence of chromium constituents over carbon activity in BCC phase. As seen by literature, it is required to make alterations in Fe-Cr-C ternary system for complete re-assessment for better mechanical data. (Alexandra. khvan *et al.*, 2014). The experimental assessments of Fe-Cr-C system up to 1984K have been studied in literature for phase's transformation. For, the temperature 973K to 1473K, the phase equilibria is found between FCC, BCC phases and carbides. Assessment predicts the BCC phase stability at 1273K and for FCC phase shows stability corresponds to 17 mole percent % of chromium atoms in the Fe-Cr-C ternary alloy system (D. Djurovic, B. Hallstedt *et al.*, 2011).The comprehensive line investigation and assessment is made for the Fe-Cr-C system for solid and solid-liquid equilibria during large composition of phases and isothermal temperature but their results are difficult to use for modeling and phase boundaries carbides. The carbon solubility in the FCC phase is again re determined and result is found higher values the previous calculations of (M.Palumbo, M. M.Selleby *et al.,* 2010).At temperature range 1173K to 1423K, the carbon solubility is studied for FCC phase with experimental shows somehow agreement with previous results for FCC phase in binary Fe-Cr system. (W. Xiong *et al.,* 2011). For alloying chromium and carbon contents, it is significant scattering for the BCC/FCC phases which need proper optimization of the system Fe-Cr-C ternary system. The thermodynamic molar activity interaction of Fe-Cr-C system is found very strongest negative deviation with carbon in steel found insoluble in BCC phase portion. (B. Hallstedt *et al.,* 2010). The high temperature deficiency in solubility of Carbon in BCC phase is studied and found the solubility of graphite phase in liquid not well operated and generated. This data could be found very useful in recent modeling of the system Fe-Cr-C ternary system. The comparison and evaluation of the Fe-Cr-C ternary system does not replace the need of the system defects and Interaction energies and metastable phases during simulation and modeling techniques by AB initio method. (Q. Chen, B. Sundman *et al.,* 2001).For industrial sectors, the need of properties erosion, abrasion and corrosion resistance are highly demanded in the group of materials as Fe-Cr-C ternary alloy system which increase the vitality and application range of the said alloy system very remarkably. The important aspects of these materials are their solidification conditions and chemical formula compositions. The hard facing alloys phases like eutectic, hypo-eutectic and microstructure of the said system are very useful in industrial sectors (C. Fan, M.C. Chen *et al.,* 2006).The phase transition and transformation of matrix from BCC to FCC is investigated above 1100K temperature with the microstructure analysis of the said alloys system. (J. Fox, S. Weisberg *et al.,* 2010).For higher percentage of chromium in the Fe-Cr –C alloy ternary system, it was predicted the appearance of Intermetallic phases just like sigma phases. The increasing content of the chromium results the carbide stability of the Fe-Cr-C ternary system. The micro hardness of the said alloy system is not linearly changes with the annealing process. The effects of annealing temperature during the rapidly solidified hypoeutectic Fe-Cr-C ternary alloys system studied by (K. Wieczerak, P. Bala

et al., 2017).The literature study on Fe-Ni-C ternary alloy system focus the main stability finding of carbon atoms in the FCC and liquid phase. The temperature manipulated for FCC stability is 1023K, 1098K, 1173K and 1323K.The solubility of carbon in the binary alloy system Fe-Ni as determined at temperature range 1580K, 1680K, and 1740K. For 1823K temperature, further investigation of the stability of Fe-Ni-C ternary system is studied by re-addition of carbon wt% .In many types of steel the graphite is found experimentally stable then cementite, but result of difficult activity is seen. The graphite is found suspended during the thermodynamic calculation of the steel by (Wenliang Liu *et al.,* 2020)

2. Procedure.

Computational methods plays an active role in the analysis of materials sciences and engineering based fields with latest approaches.properties of materials and the equilibria of phases are the processing of materials design in the scientific fields.for the proper thermodynamic discriptions and early investigations of alloys,the calphad method is the vital computational method with many databases are utilised.The hidrothermal technique of the materials design and evaluation is remarkable method for the many types of materials classifications and synthesis.The annealing may results in the crystall domains and grain sises diameter expansions(Waseem Ullah shah *et al.,* 2022; Nada Falih *et al.,* 2021; Sumaryada, T.Sofyan *et al.,* 2019)The thermocalc package databasees as developed with calphad approach and methode for variuos type of execution in experimental and theoratical value ,which based on the critical assessment and evaluation of the thermodynamic alloys system like ternary and binary systems.The most applicable techniques first principle calaculation an calphad modelling is used for getting a reliable thermodynamic rsults and simulations for BCC/FCC and HCP phases of the alloying solution.it enables the individula to make a required predictions on the certain alloys sytstems as phase formation,phase transformation,phase fraction, composition heterogenity, calculations of driving force of phases, thermal expension coefficients and molar volume data of particular alloying systems. The plotted diagrams of ternary alloys systems Fe-Ni-C/Fe-Cr-C will be analyzed studied and compared by other simulation techniques. It is one of the best simulation software and has many specialized modules for user interface with many flexible databases for Calphad (calculation of phase diagram) method. The Thermo -Calc database software will be used in order to approach and investigate quantitatively the basic effects of alloying elements particularly the effect of Fe-Ni-C/ Fe-Cr-C systems by alloying. Mechanical calculations and predictions of Meta stable ternary alloys Fe-Ni-C/Fe-Cr-C alloys system involves calculation of yielding strength, crack susceptibility coefficient ,precipitation simulations and phase transition for the given alloy system at elevated temperatures (1900-2000)K. Obtaining optimal set of thermodynamic parameters for over the whole range compositions. Base binary systems Fe-Ni/Fe-Cr with the carbon mole fraction is maintained at 0.3, 0.4, 0.5wt% and elevated temperature range of investigation for selected alloys. CALPHAD method by the inspection of existing phase diagrams will lead an effective strategy to produced accelerating discovery of new single phase high entropy alloy. PBIN database will

show extension of alloys with temperatures.(K.H LO;C.H Shek *et al.,* 2009 ; W.Xiong, Q.Chen *et al.,* 2010 ; Wei Xiong, *et al.,* 2012 ; Y.eichhammer, J.roeck, *et al.,* 2008).

3. Input for methodology

The given table shows the input for the methodology of Fe-Cr-C/Fe-Ni-C ternary simulations.

Table 1. input for the methodology of Fe-Cr-C/Fe-Ni-C ternary simulations

Composition unit	Mass percent	matrix	BCC_A_2
Temperature	1900-2000 K	Solid sol strengthening	293.15K
pressure	106 Ps	precipitate	BCC_A_2
Composition Fe	99.59	Precipitate strengthening	Simplified model
Composition Cr	0.01	Mean radius	$1.0E^{-8}$
Composition C	0.4-0.5	Critical radius	$2.88E^{-9}$
Timeout in minutes	30	kp	$7.55E^{-6}$
Scheill start temperature	2500.15K	Equilibrium strategy	Local minimization
Thermal mode	Heat flow proportional to 1/sqr(time)	Matrix phase	FCC_A_1
Liquid fraction: start for relaxation	0.6	Phase to form	M_7C_3
fraction: transition to vulnerability	0.1	Condition to vary	temperature
fraction: smallest for vulnerability	0.01	Search directions	Positive/negative
Calculation type	Grid	Phase boundary mobility	10.0 m^4/js
Mass % C/number of steps	0.0 min to 1.0 max/10	Phase energy addition	0.0j/mol
temperature	500min to 3000 max/10	Grain size/average radius	$1.0E^{-4}$m
Truncate distribution at	3 standard deviation	Dislocation density	$5.0E^{12}$
Total number of samples	200 Gaussian distributions	Molar volume	$7.0E^{-6}$
Smallest fraction	$1.0E^{-12}$	Nucleation sites	Bulk, grains
Terminate fraction phase amount	0.01	morphology	sphere

4. Thermodynamic Results/Discussion

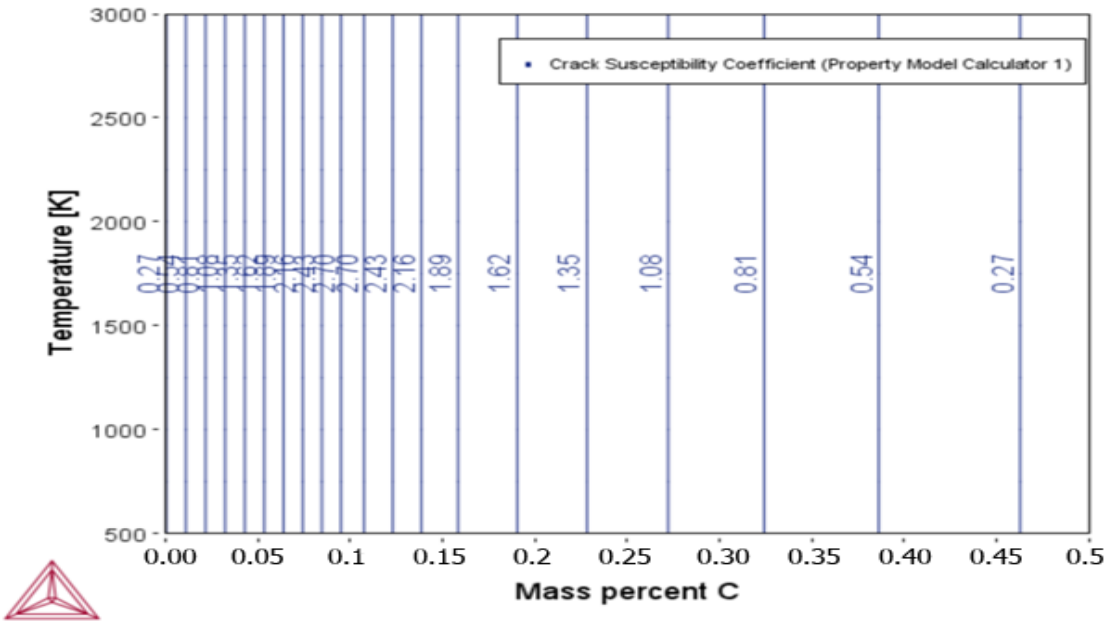

Fig. 1. (a) crack susceptibility coefficient Fe-Cr-C at elevated annealing temperature

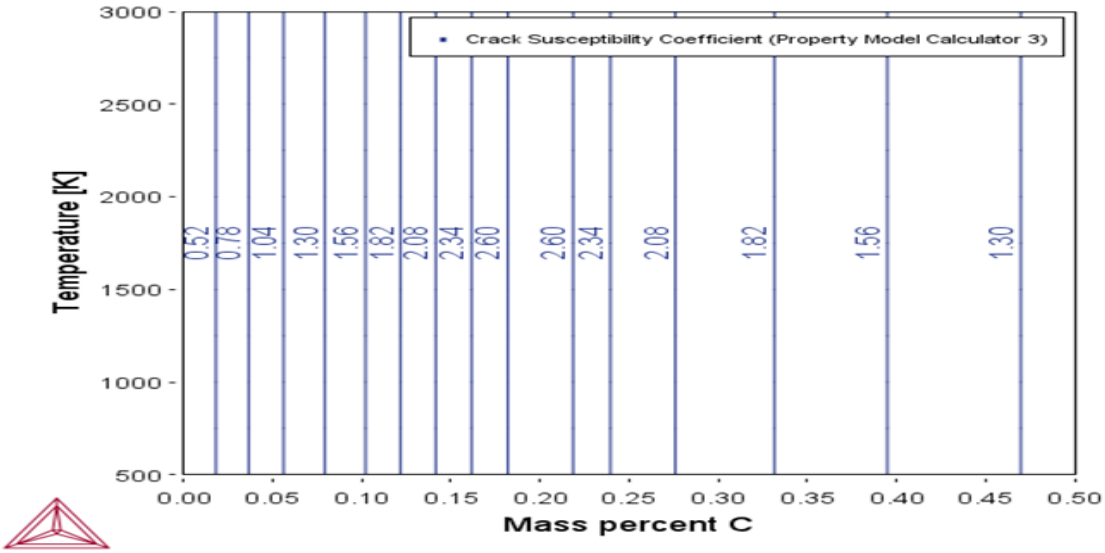

Fig. 1. (b) crack susceptibility coefficient Fe-Ni-C at elevated annealing temperature

The maximum crack susceptibility coefficient is observed of value 2.70 at the highest composition of 0.11 mass % of carbon element. The carbon composition profile in the Fe-Cr binary system gain peak value of 1.89 with the lowest soluble carbon composition of 0.152 mass%. For Fe-Ni alloys 2.60 is the maximum crack susceptibility observes at C 0.25 mass %. The susceptibility coefficient is found in-dependent on temperature but dependent on C composition. The peak value is observed 2.70 for the 0.11 mass % of carbon solubility in the Fe-Cr-C ternary system. Increasing C

composition in Ni rich section increases the crack susceptibility of the system and tends lowering the mechanical properties of Ni doped region.

Table 2. Crack Susceptibility Coefficient of Fe-Cr-C/Fe-Ni-C alloys

Crack Susceptibility Coefficient Fe-Cr-C	Crack Susceptibility Coefficient Fe-Ni-C	Mass % C/ Temperature K		Mass% Ni	Mass % Fe	Mass % Cr
0.27	0.52	0.0000	500	0.01000	99.99000	0.01000
1.89	1.04	0.0512	500	0.01000	99.94000	0.01000
2.70	1.56	0.11	500	0.01000	99.89000	0.01000
1.89	2.54	0.152	500	0.01000	99.84000	0.01000
1.08	2.60	0.25	500	0.01000	99.79000	0.01000
1.08	2.08	0.255	500	--	99.74000	0.01000
0.81	1.82	0.35	500	--	99.69000	0.01000
0.54	1.73	0.357	500	--	99.64000	0.01000
0.54	1.56	0.4000	500	--	99.59000	0.01000
0.27	1.56	0.451	500	--	99.54000	0.01000
0.27	1.30	0.452	500	--	99.49000	0.01000

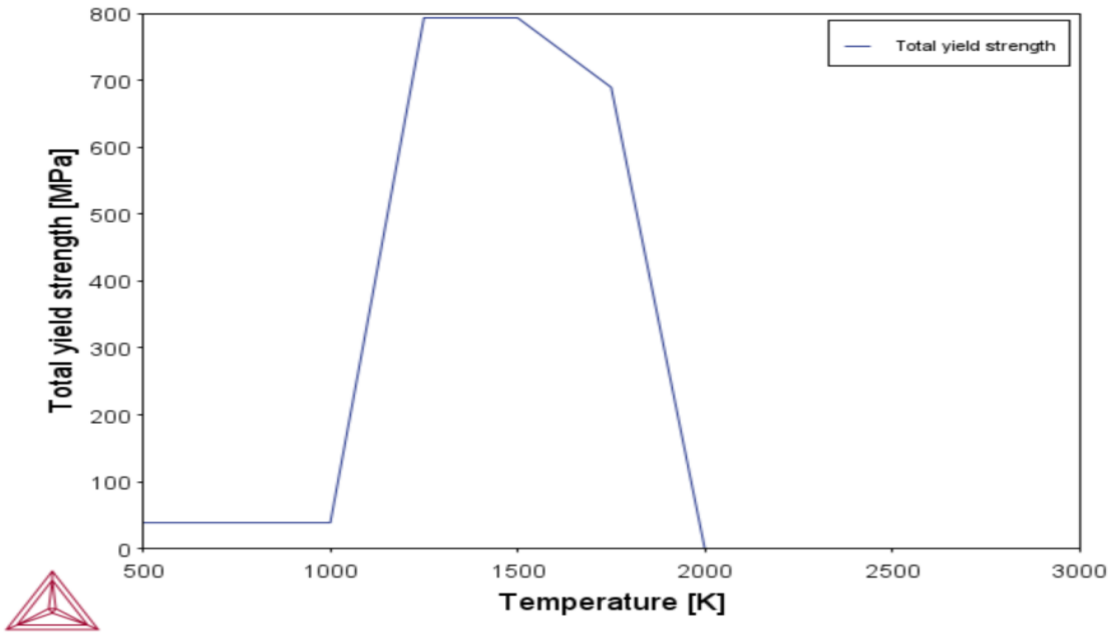

Fig. 2. (a) Yield strength variation of Fe-Cr-C system at annealing temperature with pressure 10^5 Pascal. The variations are responsive to thermal parameters and elongation of the alloying basic matrix. The fluctuations are composition dependent by varying the carbon concentration of the alloy.

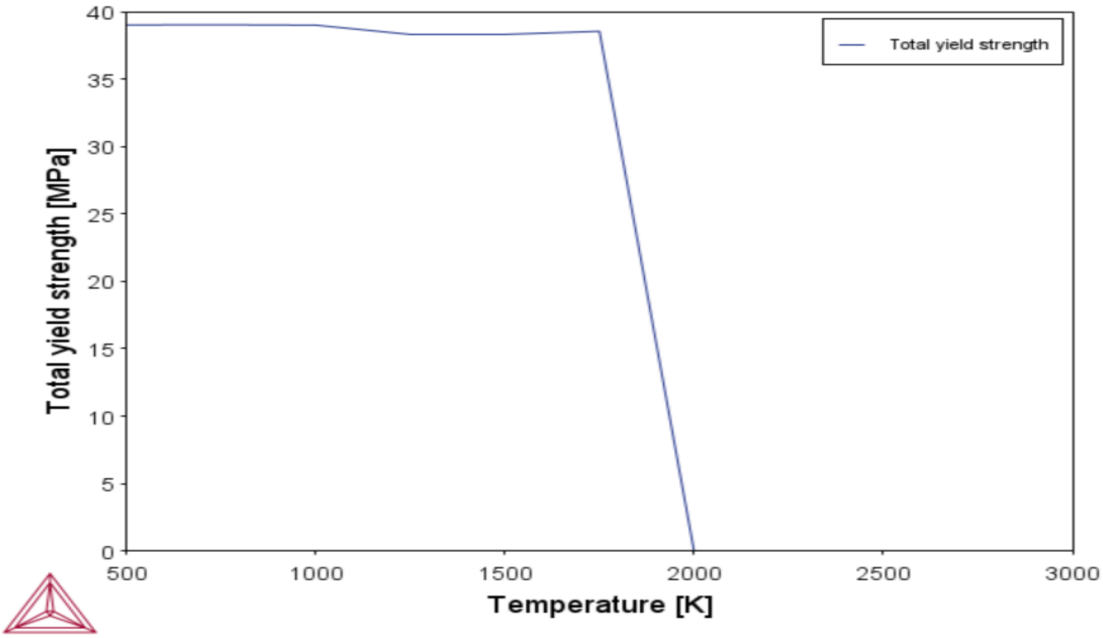

Fig. 2. (b) Yield strength Fe-Ni-C system at annealing temperature with pressure 10^5 Pascal.

For Fe-Cr-C alloy, the total yielding strength is observed 798MPa with maximum spread area of 1000-2000K temperature range. For the Fe-Ni-C system, the maximum yielding strength is observed 38MPa with the spread are of 500-2000K of temperature range. Fe-Cr-C alloy gives maximum Yielding strength with better mechanical properties. The mix ferrites and carbides formed in Cr doped matrix are creating high strength and workability of the system. The diffusion coefficients of Ni doped matrix are lower than Cr doped region, which results higher solubility of Cr rich matrix during alloying. Stacking fault energy of Ni doped matrix are found excess then Cr-doped region.

Table 3. Yielding strength Fe-Cr-C/Fe-Ni-C

Total yield strength Fe-Cr-C	Total yield strength Fe-Ni-C	Mass % C	T:^{0}K	Mass % Fe	Mass% Cr	Mass% Ni
40	38	0.0000	500-1000	99.99000	0.01000	0.01000
100	36	0	1050	99.99000	0.01000	0.01000
798	36	0.1	1250	99.99000	0.01000	0.01000
798	28	0.2	1230-	99.99000	0.01000	0.01000
670	24	0.3	1700	99.94000	0.01000	0.01000
400	5	0.4	1800	99.94000	0.01000	0.01000
40	5	0.5	1850	99.94000	0.01000	0.01000
0	0	0.55	1970	99.94000	0.01000	0.01000
		0.56	2000			

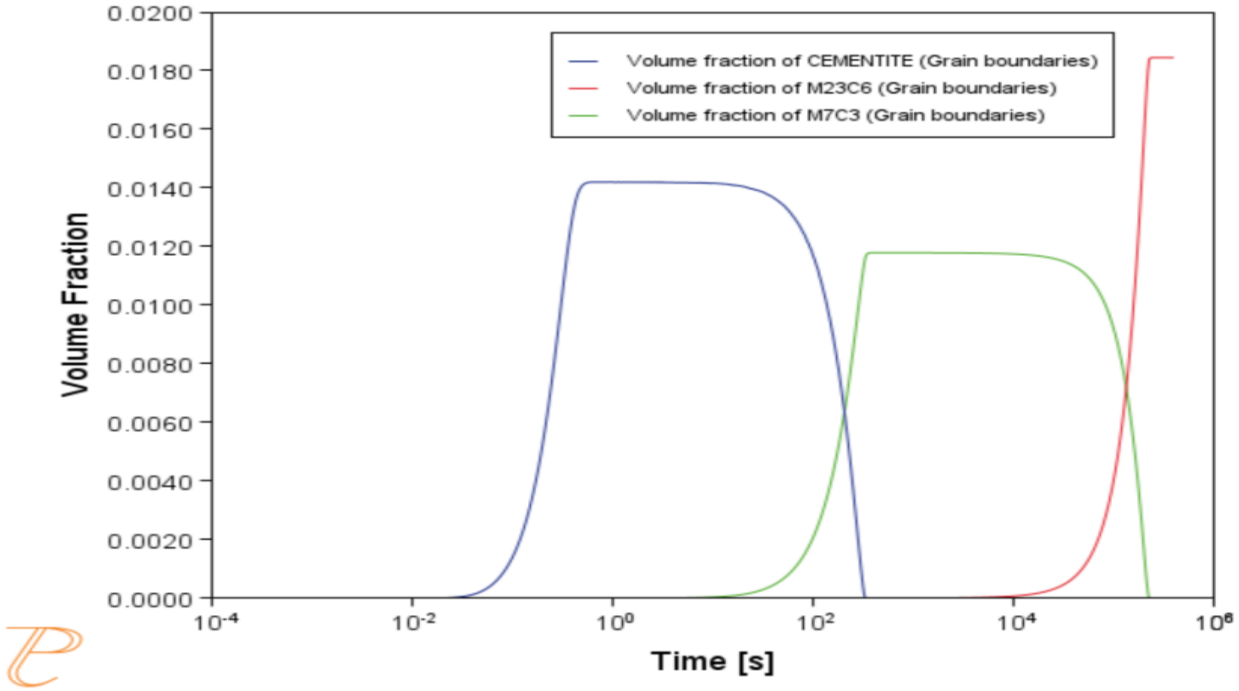

Fig. 3. (a) Precipitation from Cementite to Ferrite grain boundaries in the Fe-Cr-C alloy vs. time section.

The precipitation calculators with specific databases are found to relocates carbides and mixed carbides grains in the basic alloy matrix. Cementite grains are found low time arrow for the phases composition while $M_{23}C_6$ grains are found for the expands of more time arrow during alloying and annealing process.

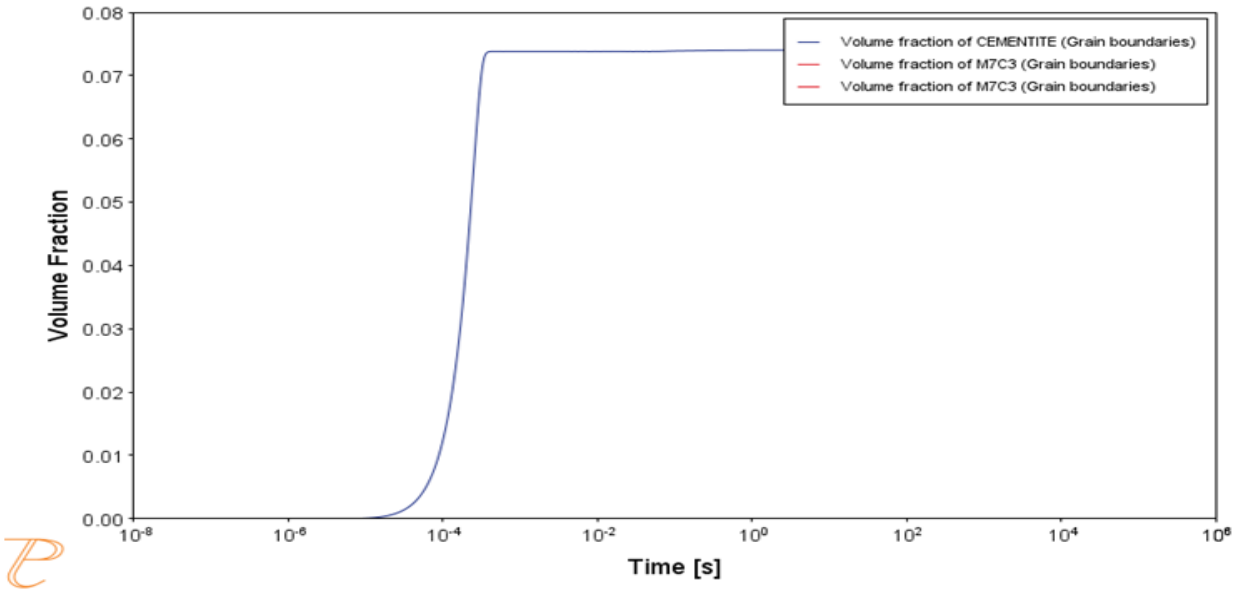

Fig. 3. (b) Precipitation from Cementite to Ferrite grain boundaries in the Fe-Ni-C alloy matrix.

The phase transition profiles of precipitate phases have studied for volume fraction verses the time axis. For Fe-Cr-C system, the peak volume fractions of the $M_{23}C_6$ grain boundary have observed with 10^4-10^5 seconds of time at X-axis and 0.000-0.0185 mass % of alloying composition. The volumetric fractions of $M_{23}C_6$ grain boundary are sharp nature with smallest spread area. The fraction of M_7C_3 grain boundary are of wide nature and the expended area from 10^1-10^5 seconds in time axis, while the volumetric fraction of the peak grain is observed from 0.000-0.0120 mass % of the alloying composition. The most expended and stable peak found for the cementite grain with 10^{-2}-10^{25} seconds of time axis and 0.000-0.0140 mass% of volumetric composition of alloying elements. For Fe-Ni-C ternary alloy, the volume fraction of cementite grain boundary is observed with maximum peal value from 0.00-0.075mass % of composition of alloying elements and the time axis is noted 10^{-4}-10^4 seconds along X-axis. The volume fractions of the M_7C_3 grain boundary are found disappeared due to the less spread and activity in the alloying. The cementite phase is recorded the most dominant and existing phase with maximum temperature surviving mode for the both ternary alloys Fe-Cr-C/Fe-Ni-C system.

Table 4. Grain boundaries with phase's transition for Fe-Cr-C/Fe-Ni-C alloys.

T:K^0	Amount of BCC_A_2	Amount of FCC_A_1	Amount of GRAPHITE	Amount of LIQUID	Amount of $M_{23}C_6$	Amount of M_7C_3	Mean radius of CEMENTITE (grain boundaries).m	Time (s)
1900-	0.00000	0.00000	0.00069	1.0000	0.01362	0.00483	$3.08590E^{-10}$	0.00011
1735	0.03040	0.16050	0.00166	1.0000	0.02495		$3.08596E^{-10}$	0.00033
1740	0.13490	0.37179	0.00261	0.83950	0.02937		$3.09165E^{-10}$	0.00033
1730	0.22130	0.52345	0.00354	0.62821	0.10924		$3.09657E^{-10}$	0.00035
1720	0.29353	0.63838	0.00445	0.47655	0.10924		$3.10094E^{-10}$	0.00039
1710	0.35451	0.72936	0.00533	0.36162	0.10924		$3.10455E^{-10}$	0.00042
1700	0.40648	0.80393	0.00619	0.27064	0.10924		$3.10868E^{-10}$	0.00047
1690	0.61420	0.86679	0.00703	0.19607	0.10924		$3.11368E^{-10}$	0.00052
1683.	0.66868	0.92103	0.00785	0.13321	0.10924		$3.12009E^{-10}$	0.00059
1680	0.69850	0.96875	0.00864	0.07897			$3.12897E^{-10}$	0.00067
1670	0.60187	1.00000	0.00941	0.03125			$3.14193E^{-10}$	0.00078
1660	0.37158	0.99931	0.01016	0.00000			$3.15866E^{-10}$	0.00092
1655.	0.19596	0.99834	0.01088				$3.18574E^{-10}$	0.00111
1650	0.13695	0.99381	0.01158				$3.23150E^{-10}$	0.00138
1640	0.11298	0.99297	0.01226			0.01228	$3.30189E^{-10}$	0.00167
1630	0.07344	0.99215	0.01291			0.01129	$3.39230E^{-10}$	0.00195
1620	0.03450	0.99136	0.01354			0.00497	$3.50435E^{-10}$	0.00223
1340-	0.00000	0.99059	0.01399			0.00817	$3.63633E^{-10}$	0.00251
1346								

Table 2-3: Shows thermodynamic calculations and results of Fe-Ni-C/Fe-Cr-C ternary system during alloying. At temperature of the range (1900-200K) the thermodynamic modeling is assessed as shown by tables 2-3 of the figures. The crack susceptibility coefficient for Fe-Cr-C is found maximum 2.83046 with a 0.2000 mass percent of carbon elements. The temperature noted here is 750K, 1000K, 1200K, 2000K, 2250K.The Fe is 99.79 mass percent with Cr of 0.1000 mass percent. The crack susceptibility coefficient for Fe-Ni-C is found maximum 0.26294 at temperature of 500K,1000K,1500K,2750K with carbon of 0.1 mass percent. Preceding results shows Fe 99.99 mass percent and Ni of 0.0100 mass percent. The yield strength of Fe-Cr-C is found maximum 824.04532 at temperature of 1750K with the carbon is substituted 0.05000 of mass percent and the Fe 99.9400 mass percent with Cr 0.01000 of mass percent. The yield strength of Fe-Ni-C is found maximum 76.74442 at temperature of 1750K with 0.3000 mass percent of carbon .The preceding results shows Fe of 99.6400 mass percent, Ni of 0.01000 mass percents respectively. The precipitation from cementite to ferrite configuration in Fe-Cr-C is found with the temperature 580K for the BCC_A_2 phase of 0.87034 mole, BCC_A1 maximum with 0.02407 mole at 580K.The liquid phase is maximum 0.82796 mole at temperature of 1730K.The FCC_A1#$_3$ phase is found maximum of 0.97063 mole at 1320K.$M_{23}C_6$ phase is seen maximum 0.10924 mole at 1660K.M_7C_3 phase is maximum 1129 mole at 1335K of temperature. The mean radius of cementite is varying from $3.08590*10^{-10}$ meter at time duration of 0.00011 seconds to $1.52642*10^{-9}$meter. For the Fe-Ni-C system, at temperature of 850K; the BCC_A2 phase is found 0.40648 moles with maximum value. The FCC_A_1 phase is found 1 mole at 1320K-1066.98K.The graphite is found maximum 0.02059 moles with 850K of temperature.

5. Conclusion

The detailed thermo-mechanical evaluation is given for the ternary alloys Fe-Ni-C/Fe-Cr-C systems by Calphad based calculations and FeDemo databases. The computational thermo-calc tool is used for all kind of modeling and simulations for the given alloys. The given thermo-mechanical calculations shows the fluctuation and optimization of the alloy system due to compositional heterogeneity .The crack susceptibility of the Fe-Ni-C is maximum then Fe-Cr-C ternary alloys, as the solubility range of carbon in the Fe-Cr-C is maximum then Fe-Ni-C alloy system. The higher crack susceptibility coefficient of the Fe-Ni-C system results the complex magnetic properties of the alloying and highest level of entropy of the system. Crack susceptibility is found independent on temperature but only dependent on C composition. The system will respond to the more quickly substitution of carbon constituents during alloying. The yielding strength of the Fe-Cr-C system is found maximum then that of Fe-Ni-C system with highest nature ferrites and carbides in the system of Fe-Cr-C. The results predicted the highest responsive mechanical and thermal properties of the Fe-Cr-C ternary alloying system. The grain boundaries of Cr doped region are stronger than that of Ni rich section. For the Fe-Cr-C system, The FCC_A1#3 phases is found maximum of 0.97063 mole at 1320K during alloying. M_7C_3 phase is maximum 1129 mole at 1335K of temperature. The mean radius of cementite is varying from $3.08590*10^{-10}$meter at time duration of 0.00011 seconds to $1.52642*10^{-9}$mater at 0.01264 seconds,

which results better precipitation simulations of the Fe-Cr-C ternary alloy system. In the Fe-Ni-C system, The FCC_A1 phase is found 1.0 mole at 1320K-1066.98K, which shows the system rare simulation with rare solubility of carbon in that particular alloy system. Activity of the system shows throughout fluctuations from the vegard,s law in positive ideal cureve,which is responsible for the complex frame of the system and rare doping characteristics greater validity for industrial variety in the system of interests and research areas .

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