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A Python Script for Calculating Magnetization in Alloys

by Efraín Hernández-Rivera, Heather A Murdoch, Anit K Giri, and Matthew C Guziewski

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14. ABSTRACT
Magnetization of a material is an important property that influences how it interacts with magnetic fields. Therefore, it is important to accurately calculate and/or predict magnetization of a wide range of material alloys. The Weiss mean field theory model and Kuz'min equation of state are explored in the technical note. Their formulations are briefly described, followed by a few examples applied to iron-based alloys. The Python module for calculating the magnetization is included as an appendix.

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magnetization, Weiss mean field theory, Kuz'min equation of state

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1. Introduction

One of the more important properties of magnetic materials is their magnetization, which influences how a material behaves when exposed to a magnetic field. For instance, it has been observed that processing under a magnetic field influences a phase's alignment and spacing[1,2] and the formation of metastable carbide precipitates.[3,4] This is a result of the magnetic field influencing the thermodynamics of the system, wherein competing kinetic and thermodynamic mechanisms are at play. The strength that a magnetic field will have on a material's behavior can be captured through the description of the thermodynamic component as a function of magnetization:

$$\Delta G_{mag}^{ext} = -\mu_0 \int_0^H M(H,T,x)dH \tag{1}$$

where μ_0 is the permeability of vacuum, H is the externally applied magnetic field, T is the processing temperature, and x is the alloy composition.

Several models (e.g., Weiss mean field theory [WMFT]) have been used to simulate and/or predict an alloy's magnetization. To fully explore some of these models, Murdoch et al. [5] performed a robust analysis and comparison of some of these models. This technical note provides some further observations on the WMFT and Kuz'min's equation of state (KEoS) models, and a more detailed description of how these models were implemented. Furthermore, the `python` class used to calculate the magnetization based on these models is included in the Appendix.

2. Model Formulations

Multiple models have been developed to predict and/or fit the magnetization of a given material. Two of these are the WMFT and Landau models, which have been successfully used to describe magnetization in a variety of materials. Here, we focus on these two models, which were recently extended to model magnetization in alloys.[5]

2.1 Weiss Mean Field Theory

WMFT denotes the magnetization of an ensemble of N atoms, each with a magnetic moment m when subjected to an externally applied magnetic field H:

$$M = mNB_j(\alpha) = M_0 B_j(\alpha) \tag{2}$$

where $M_0 = mN$ is the saturation magnetization and B_j is the Brillouin function

$$B_j(\alpha) = \frac{2j+1}{2j}\coth\left(\frac{2j+1}{2j}\alpha\right) - \frac{1}{2j}\coth\left(\frac{1}{2j}\alpha\right) \tag{3}$$

and the quantum number j is a positive integer or half-integer. The α-parameter is defined as the ratio of the Zeeman energy of the magnetic moment and the thermal energy

$$\alpha = \frac{m(H + wM)}{k_B T} \tag{4}$$

where w is the molecular field constant and k_B is the Boltzmann constant. The term wM gives the internal magnetization field. The Curie temperature, at which magnetization goes to zero in the absence of an applied external field, can be defined as

$$T_C = \frac{(j+1)wm^2N}{3jk_B}. \tag{5}$$

Since the molecular field constant can have a complex dependence on the material's electronic structure, causing it to vary widely between species, it is convenient to remove it by using Eq. 5,

$$w = \frac{3jk_BT_C}{(j+1)m^2N}, \tag{6}$$

which, by combining with Eqs. 2 and 4, we can express α as

$$\alpha = \frac{mH}{k_BT} + \frac{3jk_BT_C}{(j+1)m^2N}\frac{mM}{k_BT} = \frac{mH}{k_BT} + \frac{3jB_j(\alpha)}{j+1}\frac{T_C}{T}. \tag{7}$$

Rearranging Eq. 7, we can derive the "transcendental equation"

$$B_j(\alpha) - \frac{j+1}{3j}\frac{T}{T_C}\alpha + \frac{j+1}{3j}\frac{mH}{k_BT_C} = 0, \tag{8}$$

which must be solved numerically. This nonlinear equation was solved using the `nsolve` function of Python's `sympy` module.

2.2 Magnetization for Alloys

To properly account for alloying, the existing treatment varies the Curie temperature and magnetic moment linearly as a function of alloy composition. A description of how to extend WMFT to alloys, adopted from Guo and Enomoto,[6,7] is presented next. For example, an iron (Fe)-based material (Fe-M) has a Curie temperature given by

$$T_C^a = T_C^{Fe}(1 + a \cdot x^M) \tag{9}$$

and a magnetic moment by

$$m = m^{Fe}(1 + b \cdot x^M), \tag{10}$$

where a and b are material parameters. These material parameters can be obtained experimentally measuring how the Curie temperature and magnetic moment changes as a function of composition

$$a = \frac{100}{T_C^{Fe}} \frac{dT_C}{dx^M} \tag{11a}$$

$$b = \frac{1}{m^{Fe}} \frac{dm}{dx^M}. \tag{11b}$$

The magnetization of the binary alloy is calculated by

$$M = mNB_j(\alpha + \Delta\alpha) \tag{12}$$

where $\Delta\alpha = Ax$ is the alloying-induced change in α. Performing a first-order Taylor expansion and using Eq. 10, we get

$$\begin{aligned} M &= m^{Fe}N \cdot \left[1 + b \cdot x^M\right] \cdot \left[B_j(\alpha) + x^M A B_j'(\alpha)\right] \\ M &= m^{Fe}N \cdot \left[B_j(\alpha) + x^M A B_j'(\alpha) + b \cdot x^M B_j(\alpha) + b \cdot {x^M}^2 B_j'(\alpha)\right]. \end{aligned} \tag{13}$$

Finally, only keeping terms that depend linearly with x^M, we get

$$M = m^{Fe}N \left[B_j(\alpha) + \left\{A \cdot B_j'(\alpha) + b \cdot B_j(\alpha)\right\} \cdot x^M\right] \tag{14}$$

Examining Eq. 14, it can be observed that we still need to determine the A param-

eter. In order to derive a function for A, we can extend Eq. 8 to its alloyed form:

$$B_j(\alpha + \Delta\alpha) - \frac{j+1}{3j}\frac{(\alpha+\Delta\alpha)T}{T_C^{Fe}(1+ax^M)} + \frac{j+1}{3jk_B}\frac{m^{Fe}(1+bx^M)H}{T_C^{Fe}(1+ax^M)} = 0. \tag{15}$$

Keeping in mind that $B_j(\alpha+\Delta\alpha) = B_j(\alpha) + \Delta\alpha B_j'(\alpha)$, performing some expansion with respect to x^M and grouping by order, we get

$$0^{\text{th}}: \quad B_j(\alpha) - \frac{j+1}{3j}\frac{T}{T_C}\alpha + \frac{(j+1)mH}{3jk_BT_C} \tag{16a}$$

$$1^{\text{st}}: \quad AB_j'(\alpha) + aB_j(\alpha) - \frac{j+1}{3j}\frac{T}{T_C^{Fe}}A + \frac{(j+1)m^{Fe}Hb}{3jk_BT_C^{Fe}} \tag{16b}$$

$$2^{\text{nd}}: \quad aAB_j'(\alpha). \tag{16c}$$

Then, recognizing that $B_j(\alpha)$ corresponds to the pure alloy and combining Eq. 8 (for Fe) and the first-order terms of Eq. 16, we get

$$AB_j'(\alpha) - \frac{j+1}{3j}\frac{T}{T_C^{Fe}}(A - a\alpha) + \frac{(j+1)}{3j}\frac{m^{Fe}H}{k_BT_C^{Fe}}(b-a) = 0, \tag{17}$$

and finally, we can solve for A:

$$A = \frac{k_BTa\alpha + m^{Fe}H(b-a)}{k_BT - 3jT_C^{Fe}B_j'(\alpha)/(j+1)}. \tag{18}$$

It should be noted that once the α values for a given elemental system subjected to an applied field H are obtained, these values can be used to calculate the magnetization of the alloy based on the elemental system. Hence, we only need to calculate the α values as a function of H and T once and then reuse these for alloyed systems.

2.3 Kuz'min Equation of State

Based on Landau's theory for ferromagnets,[8] Kuz'min developed an approximate equation of state (EoS).[9] This EoS applies to ferromagnets at $T \lesssim T_C$ undergoing a second-order phase transition.

Following the ferromagnet-specific version of Landau theory, as stated by Ginzburg,[10] a thermodynamic potential can be written as an expansion of magnetization:

$$\Phi(M,H,T) = \Phi_0 + \frac{1}{2}AM^2 + \frac{1}{4}BM^4 + \frac{1}{6}CM^6 + \cdots - HM \tag{19}$$

where the coefficients $\Phi_0, A, B, C, \ldots$ may depend on external thermodynamic parameters (e.g., temperature), but not on the applied field H. Under thermodynamic equilibrium, we get

$$\frac{\partial \Phi}{\partial M} = AM + BM^3 + CM^5 + \cdots - H = 0, \tag{20}$$

which is an implicit form of the magnetic EoS, giving a relation between M, H, and T. Given the reduced magnetization ($\sigma = M/M_0$) and temperature ($\tau = T/T_C$), the magnetic EoS can be rewritten as

$$H = a\sigma + b\sigma^3 + c\sigma^5 + \cdots \tag{21}$$

where a, b, and c are functions of the reduced temperature. Kuz'min postulated that the magnetic EoS can be expressed as Eq. 21 when: 1) it has been truncated to the σ^5 term, 2) coefficients b and c are independent of τ, and 3) coefficient a dependence on τ fulfills Bloch's 3/2 power law at low temperatures:

$$a(\tau) = a_0 \frac{\tau^3 - 1}{1 + p\tau^{3/2}} \tag{22}$$

where a_0, p and $\kappa = b/a_0$ are material parameters. Then, with the normalization condition

$$\sigma(T = 0, H = 0) = 1 \qquad \rightarrow \qquad M = M_0 \tag{23}$$

we get

$$H = a_0\sigma \left[\frac{\tau^3}{1 + p + \tau^{3/2}} + \kappa\sigma^2 + (1 - \kappa)\sigma^4 \right] \tag{24}$$

where a_0, p and $\kappa = b/a_0$ are material parameters. An alternative to solving this problem, the EoS can be solved for τ:

$$\tau = \left(\sqrt{1 - 2u + p^2u^2} - pu \right)^{2/3} \tag{25}$$

where

$$u = \frac{1}{2} \left[\kappa\sigma^2 + (1 - \kappa)\sigma^4 - \frac{H}{a_0\sigma} \right]. \tag{26}$$

It should be noted that either equation could be used to fit to experimental data, where Eq. 24 can be used to fit experimental magnetization curves (σ vs. H, with fixed τ), while Eq. 26 can be used to fit temperature dependences of magnetization

at a fixed magnetic field (σ vs. τ, with fixed H).

3. Analysis of Models

This section explores how these models perform at predicting the magnetization of different metals. We consider both pure systems, and the influence of alloying through the WMFT model.

3.1 WMFT Model

WMFT has been used to calculate magnetization for pure Fe across a range of applied fields, as shown in Fig. 1. The material parameters used were obtained from Ishikawa[11] and are tabulated here for convenience (Table 1). Figure 1a shows magnetization as a function of time for multiple applied magnetic fields. As expected, for $H = 0$ T, magnetization goes to zero at the Curie temperature ($T_C = 1043$ K). We explored two cases of WMFT, where the quantum number is $j = 1/2$ (solid lines) and $j = 1$ (dashed lines). However, when subjected to an applied field, the alloy is still magnetized at temperatures over the Curie temperature. It is observed that the $j = 1/2$ case yields a magnetization that is higher than the $j = 1$ case. Figure 1b shows the percent difference between these two curves. It is shown that for small fields ($H \lesssim 10$ T), there is a sharp increase in difference when $T \sim T_C$. This difference quickly plateaus to a maximum of approximately 10%. Further, it is shown that while the difference still increases monotonically for higher applied fields, there is a substantial decrease in the difference at higher temperatures.

To determine the magnetization, we need to numerically solve Eq. 8 to obtain α at a given applied field and temperature. Since the solver requires an initial guess (α_0) for each condition, we assigned the previous temperature value to correspond to the current temperature initial guess:

$$\alpha_0^{(T+\Delta T, H=0)} \rightarrow \alpha^{(T,H=0)} \tag{27}$$

where ΔT is the temperature discretization. Whenever this discretization is too large, a numerical instability is observed as $T \rightarrow T_C$, as shown in Fig. 2. For the $\Delta T = 1$ K case, there is a large discontinuity very close to the Curie temperature. By decreasing the discretization to $\Delta T = 0.95$ K, the discontinuity is mostly gone, and for $\Delta T = 0.9$ K, no discontinuity is observed before the magnetization goes to

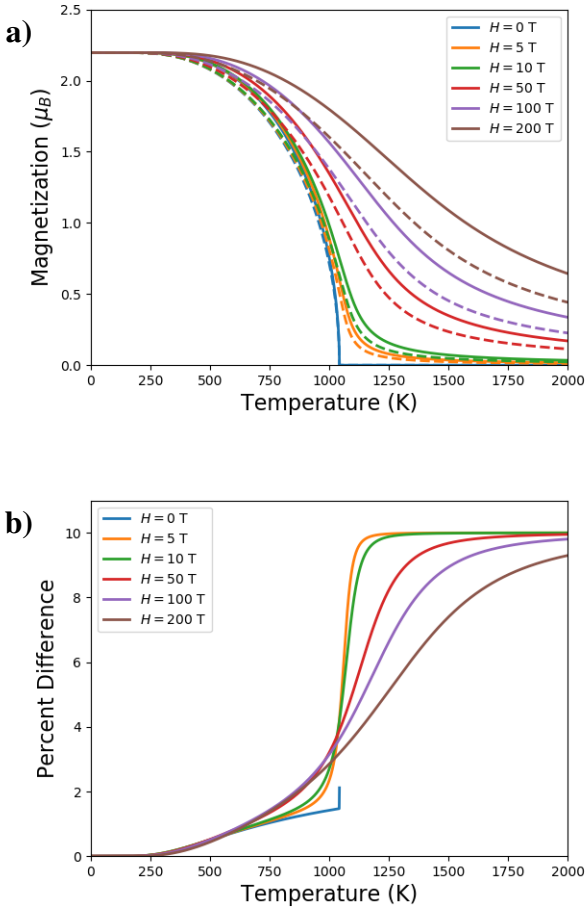

Fig. 1 Fe magnetization as calculated by WMFT, showing a) curves for $j = 0.5$ (solid) and $j = 1$ (dashed) and b) the percent difference between the different j values. This shows that the error decreases as the applied field H increases.

Table 1 Material parameters for WMFT, which describe the influence of alloying on the Curie temperature and magnetic moment in Fe (after Ishikawa[11])

Alloying element	$\boldsymbol{dT_C/dx}$ $[°C/at\%]$	$\boldsymbol{a}$	$\boldsymbol{dm/dx}$ $[\mu_B]$	$\boldsymbol{b}$
Co	12	1.15	1.11	0.5
Ni	-3.6	-0.34	1.30	0.59

$a = 100/(dT_C/dx)/T_C^0 \quad b = (dm/dx)m^{Fe}$

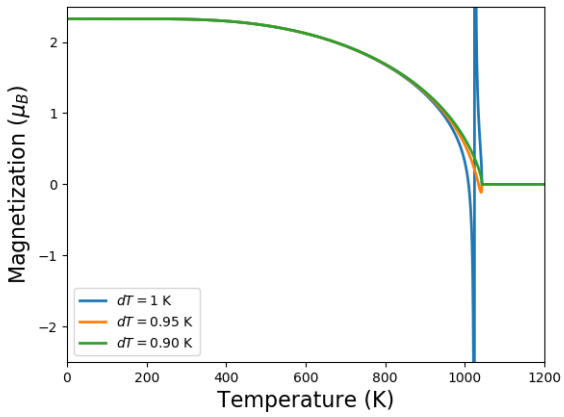

Fig. 2 Instability observed for WMFT when calculating the magnetization for the Fe–10Ni alloy

zero. It should be noted that this instability was only observed when the alloying element causes the Curie temperature to decrease ($T_C|_{x^M>0} < T_C^{Fe}$). Furthermore, this anomaly was not observed when calculating magnetization under an applied field.

Figure 3 shows the magnetization as a function of alloying composition for the Fe-cobalt (FeCo) and Fe-nickel (FeNi) systems as predicted by WMFT. It is shown that the predicted values are often not realistic, especially for high alloy content (e.g., $M_0^{x^{Ni}=0.75} > 3\mu_B$ and $T_C^{x^{Co}=0.75} \sim 1940$ K). Further, the shape of the magnetization curve is non-physical. This is likely due to the assumption that the Curie temperature and magnetic moment change linearly as a function of composition. While this might be a valid assumption for low alloying content, it is clearly not an accurate assumption otherwise, as discussed by Murdoch et al.[5]

3.2 KEoS Model

The EoS developed by Kuz'min based on Landau's theory was tested and compared against WMFT. This is shown for Fe in Fig. 4 for multiple applied magnetic fields, where the solid lines correspond to KEoS and the dashed lines correspond to WMFT. The material parameters used are shown in Table 2. Figure 4a shows that as the applied field increases the Kuz'min curves do not reach $T = 0$ K. In fact, looking at Eq. 26 and setting the reduced magnetization to one ($\sigma = 1 \rightarrow M = M_0$),

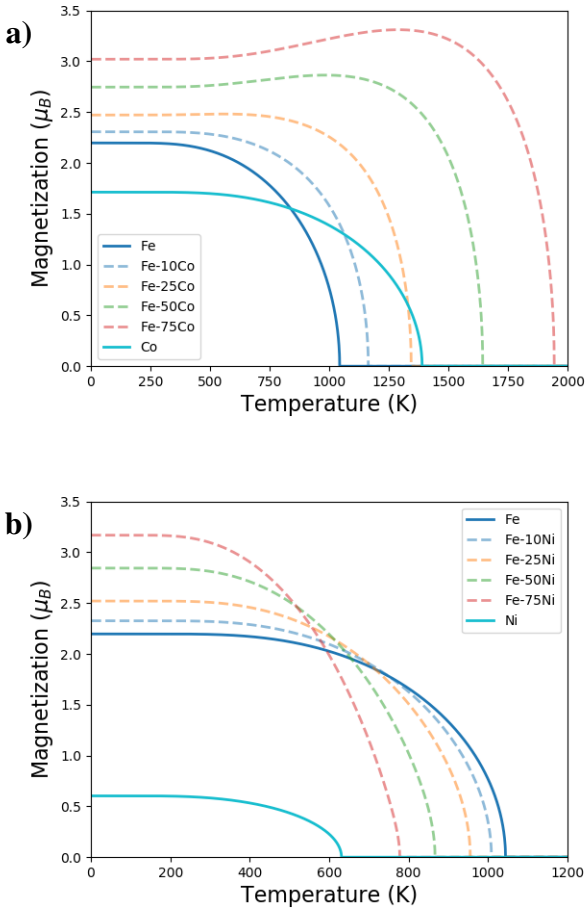

Fig. 3 WMFT prediction of magnetization as a function of alloy composition for the a) FeCo and b) FeNi systems

we get

$$u = \frac{1}{2}\left[1 - \frac{H}{a_0}\right]. \tag{28}$$

Using this equation, we can determine the temperature at which KEoS predicts that the magnetization will be saturated, as shown in Fig. 4b. We can see that as the applied field increases, KEoS becomes less practical.

Figure 5 shows the KEoS prediction of the magnetization for the FeCo and FeNi systems at different compositions. Similar to the alloyed WMFT calculations, this model is unable to accurately predict realistic magnetization and Curie temperatures. This suggests that the adjustable KEoS parameters should be refit as the al-

Table 2 Values of the parameters used for KEoS

Element	Fixed parameters		Adjustable parameters		
	M_0 (emu/g)	T_C (K)	p	κ	a_0 (MOe)
Co	164	1390	0.25	0.43	3.7
Fe	222	1043	0.25	0.18	3.3
Gd	266	293	1.5	0.35	0.9
Ni	58	631	0.28	0.47	1.85

Note: Gd = gadolinium

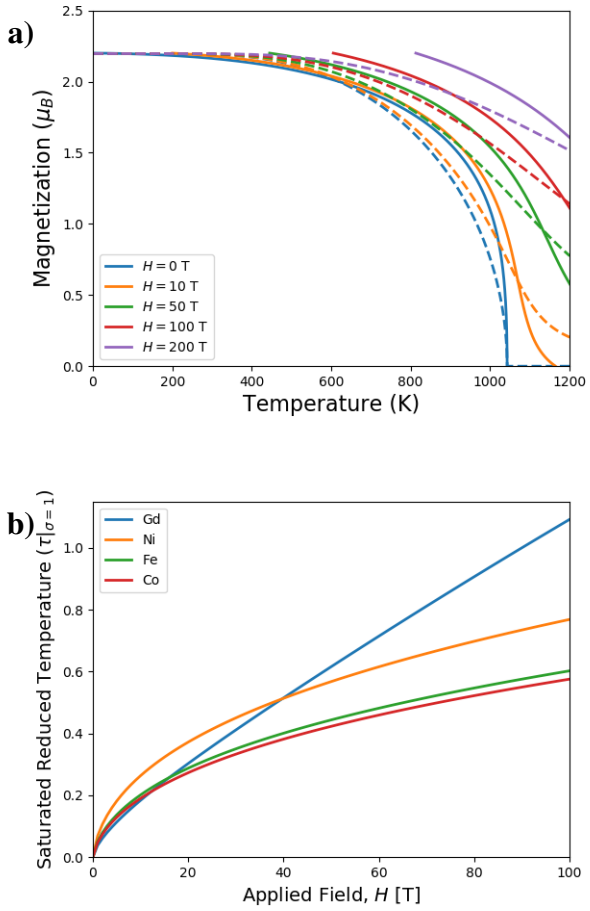

Fig. 4 Performance of KEoS in predicting magnetization of Fe. a) Comparing the Kuz'min (solid) and WMFT (dashed) models, which show that there's a limit to Kuz'min as the applied field goes up. b) reduced temperature limit at the saturation magnetization ($\tau|_{\sigma=1}$) as a function of applied field.

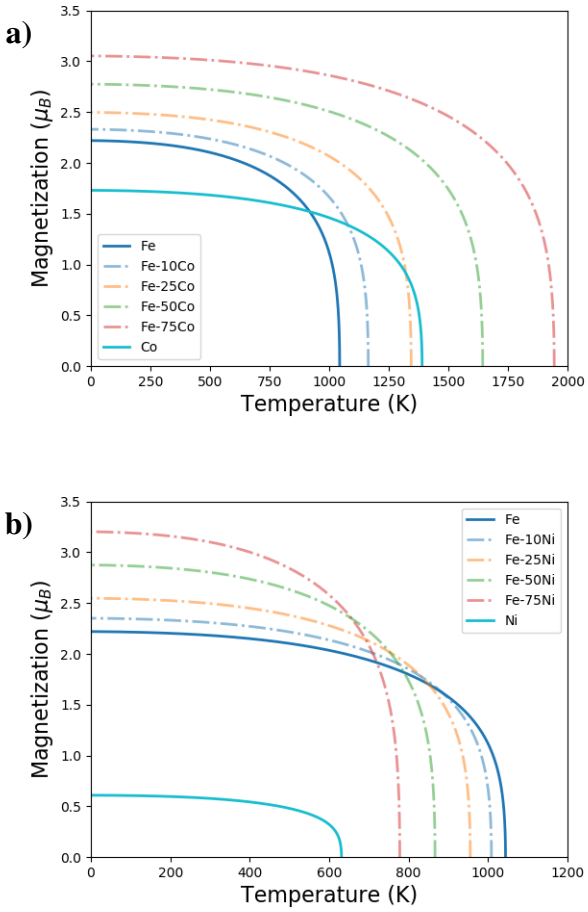

Fig. 5 KEoS prediction of magnetization as a function of alloy composition for the a) FeCo and b) FeNi systems

loys undergo phase transformations. On the other hand, the KEoS model does not show the abnormal curve shape (bump) observed for the WMFT calculations.

3.3 Model Comparison

As a final analysis, the models were used to calculate the magnetization and compared against experimental values of pure Fe,[12] Ni,[12] and Co.[13–15] The resulting calculations are shown in Fig. 6. It is clear that KEoS better approximates the magnetization for pure alloys, followed by WMFT with a half-integer quantum number ($j = 1/2$). Further, using $j = 1/2$ with applied fields would require a discontinuity at T_C to make the ferro- and paramagnetic regions consistent with their respective

descriptions under WMFT as outlined by Murdoch et al.,[5] Guo,[6] and Bozorth.[16]

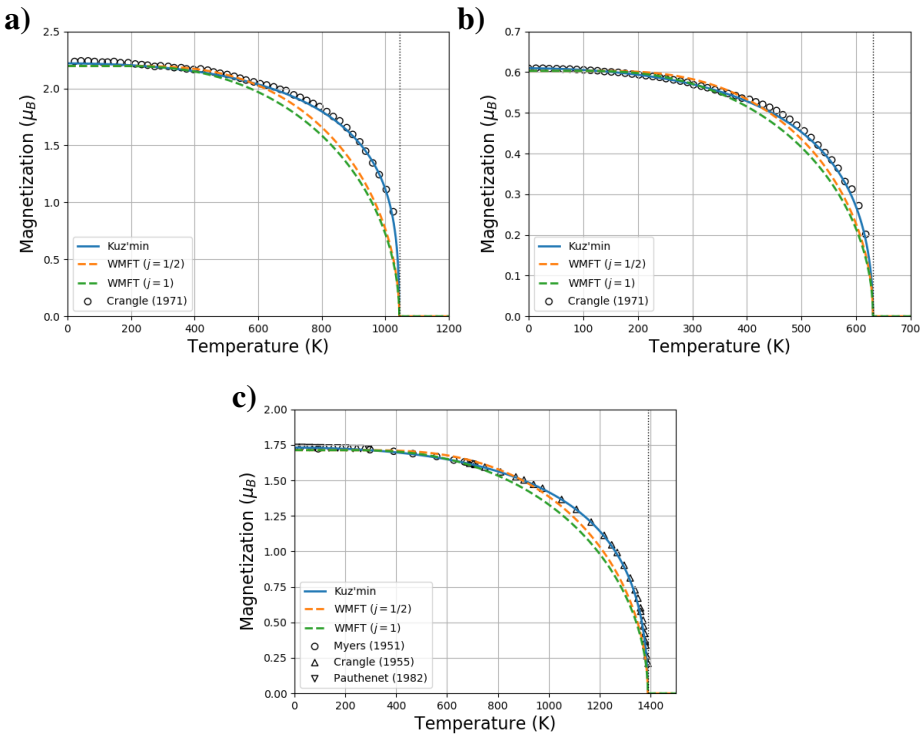

Fig. 6 Comparison between WMFT and KEoS calculated magnetization for elemental a) Fe, b) Ni, and c) Co. It is clear that Kuz'min better approximates the experimental data.

4. Conclusions

The WMFT and KEoS models were used to calculate the magnetization of metals. A numerical instability was observed for WMFT as $T \to T_C$, which depends on the temperature discretization. Furthermore, it was shown that the assumption of a linear change in the Curie temperature and magnetic moment is invalid. KEoS was shown to perform best when no applied field is present, but encounters a low-temperature limit as the applied field increases. However, it performs better than the WMFT model at predicting the magnetization of pure metals at low applied fields.

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Appendix A. Weiss Mean Field Theory (WMFT) and Kuz'min's Equation of State (KEoS) Python Script

```
'''
  ================================================================
  : class : `magnetization` -- WMFT and Kuz'min EoS magnetization
  ================================================================

  This module calculates the magnetization for a variety of alloys
    as prescribed by the WMFT and the equation of state developed
    by Kuz'min.

  Developed by Efrain Hernandez-Rivera (2019--2020)
  US Army Research Laboratory
  --
  THIS SOFTWARE IS MADE AVAILABLE ON AN "AS IS" BASIS
  WITHOUT WARRANTIES OR CONDITIONS OF ANY KIND, NEITHER
  EXPRESSED OR IMPLIED
'''

import numpy as np
from sympy import *
import matplotlib.pylab as plt

#atomic masses
Me  = {'Ni':58.6934, 'Co':58.933195, 'Fe': 55.845, 'Gd':64}

#constants
k   = 1.38e-23  # J/K
N0  = 8.49e28   # #Fe/m3
muB = 9.274e-24 # J/T

Na = 6.02214076e23
fa = 4*pi*1e-7  # funky magnetic conversion

#from Guo and Enomoto, Mat Trans JIM 41.8 911-916 (2000)
# note: a=100/Tc0*dTc/dx, b=1/mFe*dm/dx
coefs={'V': {'dTdx':7.5, 'a':0.72, 'dmdx':-2.68,'b':-1.22},\
       'Cr':{'dTdx':-1.5,'a':-0.14,'dmdx':-2.29,'b':-1.04},\
       'Mn':{'dTdx':-15.,'a':-1.44,'dmdx':-2.11,'b':-0.96},\
       'Co':{'dTdx': 12.,'a':1.15, 'dmdx':1.11, 'b':0.5},\
       'Ni':{'dTdx':-3.6,'a':-0.34,'dmdx':1.3,  'b':0.59},\
       'Mo':{'dTdx':0.,  'a':0.,   'dmdx':-2.11,'b':-0.96},\
       'Si':{'dTdx':-3.5,'a':-0.34,'dmdx':-2.29,'b':-1.04},\
       'labs':['dTc/dX','a','dm/dx','b']}

```

```
#from Kuz'min, PRB 7 184431 (2008)
# note: M0 (emu/g) Tc (K), p, kappa, a0 (MOe)
#     : 1 [emu] = 1.078283e20[uB]
#     : 1 [emu/g] * 1.078283e20 [uB/emu] * Ma [g/mol] / Na [mol/atom]
kuz  ={'Gd':{'M0':266, 'Tc':293, 'p':1.50, 'k':0.35, 'a0':0.9},\
       'Ni':{'M0':58,  'Tc':631, 'p':0.28, 'k':0.47, 'a0':1.85},\
       'Fe':{'M0':222, 'Tc':1044,'p':0.25, 'k':0.18, 'a0':3.33},\
       'Co':{'M0':164, 'Tc':1390,'p':0.25, 'k':0.43, 'a0':3.70}}

class magnetization(object):
    '''
      Class to calculate magnetization curves as a function of temperature

      Inputs:
          a, b : Coeficents for calculation of the Curie temperature and magnetic moment, respectively. Values for several alloying elements (V, Cr, Mn, Co, Ni, Mo, Si) can be called as follows:

          >>> E = 'Ni'
          >>> a, b = coefs[E]['a'], coefs[E]['b']

          [Guo and Enomoto, Mat Trans JIM 41.8 911-916 (2000)]

          Tc   : Curie temperature (K)

          H    : Magnetic field intensity (T)

          j    : Angular momentum quantum number, should be a multiple of 1/2 (optional, default=1)

          maxT : Maximum temperature (K) to which magnetization is determined (optional, default=1100)

          dT   : Discretization step for the temperature array (optional, default=0.1)

          m0   : Magnetic moment of pure iron (mu_B) (optional, default=2.2)

    '''
```

```
76
77      def __init__(self,a,b,Tc,H,j=1.,maxT=1100,dT=0.1,m0=2.22):
78          self.a  = a
79          self.b  = b
80          self.j  = j
81          self.m  = muB*m0 # [Bohr magneton]
82          self.Tc = Tc     # [K]
83          self.H  = H      # [T]
84          self.maxT = maxT # maximum T to analyze [K]
85          self.dT = dT     # temperature discretization
86
87          self.alpha, self.T = symbols('alpha T')
88
89          self.Bj  = (self.j+0.5)/self.j*coth(self.alpha*(self.j
    +0.5)/self.j)\
90                       - 0.5/self.j*coth(0.5*self.alpha/self.j)
91          self.dBj = diff(self.Bj,self.alpha)
92
93          self.alphaSol = []
94
95      def solveAlpha(self,a0=1000):
96          '''
97            Solve WMFT for pure system, obtaining alpha parameters.
     Function will loop from 1 to Tm in 1 K increments.
98
99            Inputs:
100               a0 : Initial guess for alpha (optional, default
    =1000)
101
102           Outputs:
103               alphaSol : Array of alpha values between 1 K and Tm
104         '''
105
106         j, m, alpha, T, Tc = self.j, self.m, self.alpha, self.T,
    self.Tc
107         eq = (j+1)/3./j*T/Tc*alpha - (j+1)/3./j*m*self.H/Tc/k
108         dT = np.arange(1,int(self.maxT)+1,self.dT)
109
110         for t in dT:
111             self.alphaSol.append(nsolve((eq.subs(T,t) \
112                                     - self.Bj),(alpha),(a0)))
113             a0 = self.alphaSol[-1]
114
```

```
115     def calcMag(self,X,i=0):
116         '''
117           Calculate temperature dependent magnetization for given
    alloying concentration
118 
119           Inputs:
120               X : Concentration of alloying element
121 
122           Outputs:
123               M : Array of magnetization values between 1 K and
    maxT
124         '''
125 
126         a, b, j, alpha = self.a, self.b, self.j, self.alphaSol[i]
127         m = self.m#*(1+b*X)
128         Tc = self.Tc#*(1.+a*X)
129         T = Tc*(1+a*X)*float(i)/Tc
130 
131         Bj  = self.Bj.subs( self.alpha,alpha)
132         dBj = self.dBj.subs(self.alpha,alpha)
133 
134         A = (k*T*a*alpha + (b-a)*m*self.H)/(k*T - 3.*k*self.Tc*j*
    dBj/(j+1.))
135         M = fa*m*N0*(Bj + (dBj*A + Bj*b)*X)
136         return M
137 
138     def landau(self,sig,m0=2.22,X=0.,p=0.25,k=0.18,a0=3.3):
139         '''
140           Calculate magnetization of pure Fe using Kuz'min
    application of Landau
141           [Kuz'min, Phys Rev B 77, 184431 (2008)]
142 
143           Inputs:
144               sig      : Array for the reduced magnetization (M/M0
    )
145 
146               p, k, a0 : Fitting parameters for pure Fe as
    determined by Kuz'min (optional, default= 0.25, 0.18, 3.3)
147 
148           Outputs:
149               [T, m] : Array of temperature and magnetization
    values between 1 K and Tc
150 
```

```
151
152         '''
153
154         H = self.H/1e2 #field given in T
155         u = 0.5*(k*sig**2. + (1.-k)*sig**4. - (H/(a0*(sig+1e-1))))
156         t = ((1 - 2*u + p*p*u*u)**0.5 - p*u)**(2/3.)
157
158         return np.array([t*self.Tc*(1+self.a*X), sig*m0*(1+self.b*
    X)])
159
160 if __name__=='__main__':
161     E='Ni'; dT = 0.5; maxT = 2000
162     T = np.arange(1,maxT+1,dT); n = T.size
163     m0 = kuz[E]['M0']*1.078283e20*Me[E]/Na
164     Tc = kuz[E]['Tc']
165     wmft = magnetization(0,0,Tc,0,maxT=maxT, dT=dT, j=0.5, m0=m0)
166     wmft.solveAlpha()
167     M=np.array([wmft.calcMag(0,i=i) for i in range(n)])
168
169     data = wmft.landau(np.linspace(1e-5,1,100001),p=kuz[E]['p'],k=
    kuz[E]['k'],a0=kuz[E]['a0'],m0=m0)
170
171     plt.plot(data[0],data[1],label=r"Kuz'min",lw=2)
172     plt.plot(T,M,'--',label=r'WMFT ($j=1/2$)',lw=2)
173
174     wmft = magnetization(0,0,Tc,0,maxT=maxT, dT=dT, j=1., m0=m0)
175     wmft.solveAlpha()
176     M=np.array([wmft.calcMag(0,i=i) for i in range(n)])
177
178     plt.plot(T,M,'--',label=r'WMFT ($j=1$)',lw=2)
179
180     plt.xlim(0,700)
181     plt.ylim(0,0.7)
182
183     plt.axvline(Tc,lw=1,ls=':',c='k')
184     plt.grid()
185
186     plt.xlabel('Temperature (K)',fontsize=16)
187     plt.ylabel(r'Magnetization ($\mu_B$)',fontsize=16)
188
189     plt.legend()
190     plt.show()
```

List of Symbols, Abbreviations, and Acronyms

TERMS:

Co	cobalt
Fe	iron
Ni	nickel
Gd	gadolinium
KEoS	Kuz'min's equation of state
WMFT	Weiss mean field theory

MATHEMATICAL SYMBOLS:

μ_0	permeability of vacuum
σ	reduced magnetization
τ	reduced temperature
B_j	Brillouin function
H	applied magnetic field
M	magnetization
M_0	saturation magnetization
N	atomic density
T	temperature
T_C	Curie temperature
j	quantum number
k_B	Boltzmann constant
m	magnetic moment
x	alloying composition

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