Large Scale Screening of Low cost Ferritic Steel Designs for Advanced Ultra-SuperCritical Boiler Using First Principles Methods

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Outline

- Background
- Goal
- Approach
- Project status
Background

Increasing Efficiency

Each 1% increase in efficiency eliminates ~1,000,000 tons of CO₂ emissions over the lifetime of an 800-MW plant.

US-DOE Advanced Power Systems:
46%-48% efficiency from coal generation
Steam condition: 760 °C - 35MPa
~ 5ksi

Efficiency Improvements

- Subcritical
  - 540 °C-14.5MPa
  - 35% eff.
  - mature technology
- Supercritical
  - current market introduction
  - 600 °C-28MPa

MATERIALS WITH INCREASED
CREEP & OXIDATION RESISTANCE
100,000hr Creep-Rupture for USC Boiler Materials

- Ferritic Steels (9-12Cr)
- Austenitic Alloys
- Nickel-Based Superalloys

Temperature (°C) vs. 100,000hr Creep-Rupture Stress (MPa)

- SAVE 12
- CCA617
- Std. 617
- Inconel 740
- Haynes 230
- HR6W

Dashed Line is Projected Value
Material requirements for Advanced Ultra-SuperCritical (AUSC) boiler:

- **Low cost** metal
- Compatible thermal properties
- Sufficient high temperature performance
  - Sufficient mechanical strength
  - Creeping resistance
  - Corrosion resistance
- **Low temperature ductility**
Motivation

- Ferritic steel
  - BCC matrix with low Ni content (low cost)
  - Low temperature brittleness
  - Weldability

- New design of ferritic steel
  - Composition modulation
  - Microstructure engineering
Complexity of the Alloy Strategy

- Many structural factors:
  - Matrix
  - Precipitation
  - Grain boundary
  - Interphase

- Correlated problem
  - Doping may solve a problem but bring in more problems
  - Difficult to assess the effect of alloying
# Known 9-12% Cr Ferritic Steels

Table 1. Precipitate Phases in Different Steel Phases. PT Represent for Prototype Structure and SG for Space Group Number.

<table>
<thead>
<tr>
<th>Precipitate Phase</th>
<th>PT</th>
<th>SG</th>
<th>P91</th>
<th>P92</th>
<th>E911</th>
<th>AXM</th>
<th>HCM12</th>
<th>P122</th>
<th>T122</th>
<th>NF12</th>
<th>FN5</th>
<th>TB12</th>
<th>VM12</th>
<th>X20</th>
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<tbody>
<tr>
<td>BCC_A2</td>
<td>W</td>
<td>229</td>
<td>X</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
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<tr>
<td>M23C6</td>
<td>Cr23C6</td>
<td>225</td>
<td>X</td>
<td>x</td>
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<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
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<tr>
<td>LAVES</td>
<td>MgZn2</td>
<td>194</td>
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<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
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</tr>
<tr>
<td>Z_PHASE</td>
<td>NaCl</td>
<td>225</td>
<td>X</td>
<td>x</td>
<td>x</td>
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<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
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<tr>
<td>NbNi3</td>
<td>Al3Ti</td>
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<td>X</td>
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<td>x</td>
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<td>x</td>
<td>x</td>
<td>x</td>
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<tr>
<td>AlN</td>
<td>ZnO</td>
<td>194</td>
<td>X</td>
<td>x</td>
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<td></td>
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<tr>
<td>SIGMA</td>
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<td></td>
<td>x</td>
<td></td>
<td>x</td>
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<td></td>
<td></td>
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<tr>
<td>FCC_A1</td>
<td>Cu</td>
<td>225</td>
<td>x</td>
<td>x</td>
<td>x</td>
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<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
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<tr>
<td>HCP_A3</td>
<td>Mg</td>
<td>194</td>
<td>x</td>
<td>x</td>
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<td></td>
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<tr>
<td>M2B_tet</td>
<td>Fe2B</td>
<td>140</td>
<td>x</td>
<td></td>
<td></td>
<td></td>
<td>x</td>
<td></td>
<td></td>
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<tr>
<td>MU_PHASE</td>
<td>W6Fe7</td>
<td>166</td>
<td>x</td>
<td></td>
<td></td>
<td></td>
<td>x</td>
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<tr>
<td>M6C</td>
<td>W3Fe3C</td>
<td>227</td>
<td>x</td>
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<td></td>
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<tr>
<td>Cr2B_ortho</td>
<td>Mg2Cu</td>
<td>70</td>
<td></td>
<td></td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
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<tr>
<td>PI</td>
<td>Mo3Al2C</td>
<td>70</td>
<td>x</td>
<td></td>
<td></td>
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<td></td>
<td>x</td>
<td>x</td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 1. Precipitate Phases in Different Steel Phases. PT Represent for Prototype Structure and SG for Space Group Number.
Ferritic Steel Matrix

- **BCC structure**

- **Composition of the BCC matrix in 9-12% Cr steels**

<table>
<thead>
<tr>
<th>Name</th>
<th>Fe</th>
<th>Cr</th>
<th>Ni</th>
<th>Mo</th>
<th>Si</th>
<th>Al</th>
</tr>
</thead>
<tbody>
<tr>
<td>P91</td>
<td>0.9898</td>
<td>5.87E-4</td>
<td>8.42E-9</td>
<td>6.64E-3</td>
<td>2.77E-3</td>
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<tr>
<td>E911</td>
<td>0.9969</td>
<td>5.29E-4</td>
<td>1.13E-8</td>
<td>2.03E-3</td>
<td>5.75E-12</td>
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<tr>
<td>P92</td>
<td>0.9944</td>
<td>5.55E-4</td>
<td>2.30E-8</td>
<td>3.83E-3</td>
<td>6.14E-4</td>
<td></td>
</tr>
<tr>
<td>AXM</td>
<td>0.9964</td>
<td>5.45E-4</td>
<td>1.97E-7</td>
<td>1.31E-3</td>
<td>1.15E-3</td>
<td></td>
</tr>
<tr>
<td>HCM12</td>
<td>0.9977</td>
<td>5.36E-4</td>
<td>1.19E-8</td>
<td>1.72E-3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P122</td>
<td>0.9986</td>
<td>5.15E-4</td>
<td>1.08E-11</td>
<td>2.99E-4</td>
<td>4.18E-11</td>
<td></td>
</tr>
</tbody>
</table>
Objectives

- Screening ferritic steel design based on properties of the solid solution matrix
  - Elastic properties
  - Low temperature ductility

- Develop efficient parallel software for large scale screening calculations
  - First principles quality for solid solution system
  - Automated solid solution structure sampling
  - Automated properties calculations
Approach: Structure Modeling

- Dilute multi-component solid solution
  - requires huge atomic structure model
  - components of very low concentration considered as point defect

- Special quasi-random structures
Properties calculations

- **Supercell Approaches**
  - Ensemble Average of Supercells:
    \[ F(\vec{\sigma},T) \approx \sum_{i \in \vec{\sigma}} w_i(T) F_i(T) \]
    
    superscells are local snapshots in the infinite solid solution lattice \( \vec{\sigma} \)

- **Cluster Expansion Methods**
  - Weighted average of clusters:
    \[ F(\vec{\sigma},T) \approx \sum_{\alpha,s} K^s_{\alpha}(T) \Phi^s_{\alpha} \]
    
    \( \alpha,s \) are cluster indices and cluster order indices
    clusters are local structures in the infinite solid solution lattice \( \vec{\sigma} \)
  - Mathematically rigorous
Cluster Expansion Method for multi-component multi-sublattice systems:

\[ F(\vec{\sigma}, T) \cong \sum_{\alpha,s} K_{\alpha}^{s}(T) \Phi_{\alpha}^{s}, \]

\[ \Phi_{\alpha}^{s} = \prod_{i} \Phi_{\beta_{i}}^{s_{i}}; \alpha = \bigcup_{i} \beta_{i} \]

**Challenge:** number of cluster expansion terms \( n \)

\[ n \sim (N - 1)^{\alpha |N_{\text{sublattice}}} \]

**UnitCell Expansion Method for multi-component multi-sublattice systems:**

\[ F(\vec{\sigma}, T) \cong \sum_{\gamma,s} K_{\gamma}(T) \Phi_{\gamma}^{s}, \]

**Rationale:** Coarse grained cluster (CGC) expansion,
- Unitcells are treated as pseudo atom types
- Simplify lattice
- Expected must faster cluster interaction decaying over distance (up to pair)
- Much larger number of components (pseudo atoms) (unitcell types)
Special Quasirandom Structure

- Poor man’s approximation to cluster expansion method

\[
F(\bar{\sigma}, T) \approx \sum_{\alpha, s} K^s_{\alpha}(T) \Phi^s_{\alpha},
\]

\[
\langle F \rangle_{SQS} \approx \sum_{\alpha, s} K^s_{\alpha}(T) \langle \Phi^s_{\alpha} \rangle_{SQS},
\]

\[
\langle \Phi^s_{\alpha} \rangle_{SQS} \approx \langle \Phi^s_{\alpha} \rangle
\]
At high temperature limit
- site occupation is complete random
- correlation function is known

\[ \rho_\alpha (\sigma_{HT}) = \prod_{i \in \alpha} \left\langle \gamma_{\alpha_i, M_i} (\sigma_i) \right\rangle_\alpha \]

- match SQS correlation with the known correlation function
  - Exhaustive search
  - Genetic algorithm
  - Other global optimization approach may also be used
B. Application to 9-12Cr Ferritic Steels

- B.1 Properties of known 9-12Cr ferritic steel
  - Positive control using well characterized 9-12Cr ferritic steels
    - P91, E911, P92, AXM, HCM12, P122, T122, NF12, FN5, TB12, VM12 and X20
  - Formation energy and Elastic constants will be assessed initially.
  - Assess ductility using the ratio of bulk modulus and shear modulus.
  - Stacking fault energy and surface cleavage energy will be carried out to estimate the Rice-Thomson parameter which is widely used as ductility criterion.
  - Trend analysis of indicative parameter of ductility.
**B. Application to 9-12Cr Ferritic Steels**

- **B.2 Screening studies of Ferritic Steels**
  - Screening in a progressive manner with 4 components BCC solid solutions examined first.
  
    - Precipitation effects to be assessed through homogenization
  
    - Global optimization methods such as simulated annealing and genetic algorithm to locate the optimal ferritic design.
Challenges In Structure Modeling

- Incomplete structure information about the phases in the steel
  - Missing information about site distribution
  - Phase compositions are known
  - Multiple non-equivalent solid solution sites

- Composition requires exceedingly large model
  - Dopant concentration between 1000ppm to 1ppm
    - Need to assess the dopant-dopant interaction
    - Model requires > 1000 atoms
  - Dulite dopant can be treated as point defect
  - Using the scaling law to estimate the effect of dopant with intermediate concentration: $G \sim c^\alpha$
<table>
<thead>
<tr>
<th>Phase</th>
<th>Vol fract</th>
<th>Composition</th>
<th>Crystal</th>
<th>Microstructure</th>
</tr>
</thead>
<tbody>
<tr>
<td>BCC-A2#2</td>
<td>0.8464</td>
<td>Fe$<em>{0.996}$Si$</em>{0.002}$Al$_{0.001}$</td>
<td>cI2</td>
<td>Matrix phase</td>
</tr>
<tr>
<td>BCC-A2#1</td>
<td>0.1006</td>
<td>Cr$<em>{0.957}$Mn$</em>{0.043}$</td>
<td>cI2</td>
<td>Precipitation</td>
</tr>
<tr>
<td>M$_{23}$C$_6$</td>
<td>0.0203</td>
<td>(Cr$<em>{0.864}$Mn$</em>{0.130}$Fe$<em>{0.006}$)$</em>{23}$C$_6$</td>
<td>cF116</td>
<td>Precipitation</td>
</tr>
<tr>
<td>μ-Phase</td>
<td>0.0112</td>
<td>(Fe$<em>{0.992}$Cr$</em>{0.008}$)$<em>7$(W$</em>{0.650}$Mo$_{0.35}$)$_6$</td>
<td>hR39</td>
<td>Precipitation</td>
</tr>
<tr>
<td>FCC-A1#1</td>
<td>0.0100</td>
<td>Ni$<em>{0.584}$Fe$</em>{0.370}$Si$_{0.046}$</td>
<td>cF4</td>
<td>Precipitation</td>
</tr>
<tr>
<td>M$_6$C</td>
<td>0.0037</td>
<td>(Mo$<em>{0.992}$W$</em>{0.008}$)MoFe$_2$C</td>
<td>cF112</td>
<td>Precipitation</td>
</tr>
<tr>
<td>Z-Phase</td>
<td>0.0051</td>
<td>(Cr$<em>{0.898}$Fe$</em>{0.102}$)VN$_{0.669}$</td>
<td>tP6</td>
<td>Precipitation</td>
</tr>
<tr>
<td>NbNi$_3$</td>
<td>0.0010</td>
<td>Ni$_3$Nb</td>
<td>oP8</td>
<td>Precipitation</td>
</tr>
<tr>
<td>AlN</td>
<td>0.0012</td>
<td>AlN</td>
<td>hP4</td>
<td>Precipitation</td>
</tr>
<tr>
<td>FCC-A1#3</td>
<td>0.0003</td>
<td>Cu$<em>{0.999}$Ni$</em>{0.001}$</td>
<td>cF4</td>
<td>Precipitation</td>
</tr>
<tr>
<td>M$_2$B</td>
<td>0.0003</td>
<td>(Mo$<em>{0.953}$Cr$</em>{0.047}$)$_2$B</td>
<td>tI12</td>
<td>Precipitation</td>
</tr>
</tbody>
</table>
Structure Modeling

Composition

$A_xB_yC_z \ldots$

Structure Prototype

Space group

Wyckoff site $i$

$[A_{xi}B_{yi}C_{zi}]_1$

$[A_{xi}B_{yi}C_{zi}]_i$

Total composition

Wyckoff site composition

Lattice site occupation

SQS Models

Lattice Site

Occupation $\sigma_i$

$A_1$

$B_i$

$\ldots$

$\ldots$
Structure Modeling

- **Structure models generation**
  - Based on structure prototype
  - Limited to size < 250 atoms
  - Site-distribution based on prior knowledge

- **Composition requires exceedingly large model**
  - Dopant concentration between 1000ppm to 1ppm
  - Need to assess the dopant-dopant interaction
  - Model requires > 1000 atoms
  - Dulite dopant can be treated as point defect
  - Using the scaling law to estimate the effect of dopant with intermediate concentration: \( G \sim c^\alpha \)
Elastic Constants Calculations

- Calculated use the in-home developed G(p,T) package
  - Employed VASP as the computing engine
  - Automate the calculation and fully taking advantages of symmetry
  - Both stress and energy based calculations are available

- Accuracy setting:
  - Standard 400eV energy cutoff
  - Standard K-point sampling: metal (cutoff 35), others (cutoff 25)
  - Energy convergence $10^{-6}$ eV
  - Spin polarized calculation for selected phases
## Elastic Constants Calculations

<table>
<thead>
<tr>
<th>Phases</th>
<th>$C_{11}, C_{22}, C_{33}$</th>
<th>$C_{44}, C_{55}, C_{66}$</th>
<th>$C_{12}, C_{13}, C_{23}$</th>
<th>K</th>
<th>G</th>
<th>E</th>
<th>v</th>
<th>G/K</th>
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<tbody>
<tr>
<td>BCC-A2#1</td>
<td>376 433</td>
<td>42 73</td>
<td>232 135</td>
<td>239</td>
<td>67</td>
<td>185</td>
<td>0.371</td>
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<tr>
<td>BCC-A2#2</td>
<td>330 estimated</td>
<td>110 estimated</td>
<td>171 estimated</td>
<td>224</td>
<td>97</td>
<td>253</td>
<td>0.311</td>
<td>0.433</td>
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<td>AlN</td>
<td>377 356</td>
<td>113 125</td>
<td>129 99</td>
<td>196</td>
<td>122</td>
<td>304</td>
<td>0.241</td>
<td>0.622</td>
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<tr>
<td>FCC-A1#1</td>
<td>322 147</td>
<td>179</td>
<td>225 106</td>
<td>275</td>
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<td>Cu</td>
<td>181 83</td>
<td>121</td>
<td>140 56</td>
<td>147</td>
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<td>0.399</td>
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<td>$M_{23}C_6$</td>
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<td>216</td>
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<td>0.328</td>
<td>0.388</td>
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<td>$M_2B$</td>
<td>440 141</td>
<td>199</td>
<td>282 137</td>
<td>353</td>
<td>0.291</td>
<td>0.486</td>
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<tr>
<td>$M_6C$</td>
<td>442 115</td>
<td>203</td>
<td>282 117</td>
<td>308</td>
<td>0.318</td>
<td>0.413</td>
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<td>$\mu$-phase</td>
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<td>245 225 217</td>
<td>293 95 256</td>
<td>0.354</td>
<td>0.323</td>
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<tr>
<td>NbNi$_3$</td>
<td>290 113</td>
<td>178</td>
<td>206 91 238</td>
<td>0.307</td>
<td>0.442</td>
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</tr>
<tr>
<td>Z-phase</td>
<td>278 45 167</td>
<td>189 29 83</td>
<td>0.427</td>
<td>0.154</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Precipitation Effects

- Homogenization scheme to assess the precipitation effects on elastic constants
  - Eshelby’s inclusion theory
Effective Self Consistent Scheme

- Iterative scheme
- Multiple inclusion phases allowed
- Only volume fraction and bulk elastic constants used in the scheme

\[ C^* = (H + C_M^{-1})^{-1} \]

\[ H = \sum (H_{l,i} d (I - \Omega_{DI,i} H))^{-1} \]

\[ H_{l,i} d = c_i \{ (C_{l,i}^{-1} - C_M^{-1})^{-1} + C_M(I - S_{l,i} M) \}^{-1} \]

\[ \Omega_{DI,i} = C^*(I - S_{l,i}^*) \]
Elastic properties of AXM steel

- Homogenized elastic modulus
  - Bulk modulus = 228 GPa,
  - Shear modulus = 94 GPa
  - Young’s modulus = 249 GPa
  - Poisson’s ratio = 0.318
Inverse: Properties $\rightarrow$ Structure

- First principles method brings chemical accuracy for properties calculation with known structure

- The inverse process from properties to predict structure remains the greatest challenge to material science

- Two-step approach/Material genome approach
  - Properties $\rightarrow$ Composition $\rightarrow$ prototype library
Ordered lattice structures:

- Crystal and Solid Solution
- Common description: \( \{ L_i \} \otimes \{ r_j; \sigma_j \} \)
  
  \( \{ L_i \} \) is the set of lattice symmetry operators
  \( \{ r_j \} \) is the set of lattice basis
  \( \{ \sigma_j \} \) is the set of composition vector

Composition vector \( \sigma \)

- \( \sigma = \sum_i \eta_i \varepsilon_i \)
- Each vector basis \( \varepsilon_i \) represents an element or a structure unit
- The component \( \eta_i \) represents the probability of the basis at the site
- Vacancy is also a basis
Material Genome Approach
- The challenge is how to traverse the enormous configuration space
- Uniform structure indices are highly desired for data mining

LatMGA: separate lattice from composition
- Structure = \{ L_i \} \otimes \{ r_j; \sigma_j \} = \{ L_i \} \otimes \{ r_j \} \oplus \{ L_i \} \otimes \{ \sigma_j \}
- Structure is indexed by lattice prototype and composition type
- Observation: any lattice basis sets is a subset of a fine grid inside the unit cell. For any stable structure at room temperature, the grid needs not to be finer than the range of atomic vibration. Therefore, any lattice may be a subset of supercell of a simple lattice such as simple cubic and hexagonal.
LatMGA:

- A systematic approach to index structure prototype
  - { # lattice prototype
  - { lattice unit type<scc,hcp, etc.>,
  - supercell <nxnxn>,
  - space group }
  - # composition space
  - { mask vector,
  - composition vectors }
  - }

- Three stage material configuration space exploration
  { lattice prototype discovery: 
  traverse the structure prototype indices; }
  { composition space discovery: 
  rules based selection of mask/composition vectors; 
  combine with lattice prototype to produce structure sample; 
  structure sample can be evaluated using first principles methods; }
  { material genome approach: 
  big data analysis on the high dimension structure indices space; 
  inverse map from properties to structure; }
Z-phase indices:

** it is a subset of 2x2x8 supercell of 1 basis simple cubic lattice casted into space group 129

Composition:
\[ \varepsilon_1 = \text{Nb}, \quad \varepsilon_2 = \text{V}, \quad \varepsilon_3 = \text{Cr}, \quad \varepsilon_4 = \text{N}, \quad \varepsilon_5 = \text{Vac} \]

- Site_1: \( (0.5, 0.5, 0, 0, 0) \)
- Site_2: \( (0, 0, 1, 0, 0) \)
- Site_3: \( (0, 0, 0, 1, 0) \)

Lattice prototype:

- space group: 129 (P4/nmm)
- irreducible sites:
  - Site_1: 2c 1/4 1/4 7/8
  - Site_2: 2c 1/4 1/4 5/8
  - Site_3: 2c 1/4 1/4 1/8

### casted from scc-2-2-8 to 129 :: size= 2 2 8 ###

<table>
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<tr>
<th>Site</th>
<th>( x )</th>
<th>( y )</th>
<th>( z )</th>
<th>#</th>
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<td>0.00000</td>
<td>2  a Aa</td>
</tr>
<tr>
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<td>0.25000</td>
<td>0.87500</td>
<td>4 f Ab</td>
</tr>
<tr>
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<td>0.25000</td>
<td>0.75000</td>
<td>4 f Ac</td>
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<td>0.62500</td>
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</tr>
<tr>
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<td>0.50000</td>
<td>2 b Ae</td>
</tr>
<tr>
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<tr>
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<td>2 c Al</td>
</tr>
<tr>
<td>Am1</td>
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<td>0.25000</td>
<td>0.87500</td>
<td>2 c Am</td>
</tr>
</tbody>
</table>
Progress:

- Tested against all cubic phases found in the Crystallography Open Database

- Excluding wrongful data, all can be indexed using supercell of simple cubic casted into the specific space group and a mask to indicate the closely matched Wyckoff sites (for example, Ag1, Ak1, Am1 sites, a mask vector [0 0 0 0 0 1 0 0 0 1 0 1])

- We are now in the process of implementing programs to search for unexplored masks by combining with basis information of atoms such as atomic size, charge, etc.
Progress:

- All cubic phases with space group 225 (total 689 valid structures)
  - 304 mapped to SCC-2-2-2
  - 229 mapped to SCC-4-4-4
  - 10 mapped to SCC-6-6-6
  - 133 mapped to SCC-8-8-8
  - 13 mapped to SCC-12-12-12
Future Plan

- Study mechanical properties of all phases found in the 9-12% Cr ferritic steels;
- Search for steel composition with improved mechanical properties.

Development of the LatMGA method for:
- Prototype library generation based on composition
- Automate structure model generation based on prototype library
- Automate the properties calculation of structure models
- Data mining to map properties to composition