8.3 Syntax and Examples of Phase-Field Database File (.PFDB)

The phase-field database file (.pfdb) uses the XML format, which defines the phase-field model related parameters as well as physical properties for each phase. Phase-field model related parameters include order parameter mobility, chemical gradient term, smoothness factor, driving force scaling factor, interface width, chemical random amplitude, chemical gradient factor and so on. Physical parameters of each phase include molar volume, stiffness tensor, chemical misfit strain, stress-free transformation strain, interfacial energy and so on. Nucleation related parameters can also been set through .pfdb file. The database file is designed for easy extension when user uses a customized phase-field model plugin.

In a .pfdb file, a series alloys can be defined. Each alloy has a matrix phase with one or multiple precipitate phase. User can define new types of phases when models other than precipitation are used as plugin. A sample .pfdb file structure is shown as follows,

```
<Alloy name="AlNi_Precipitation">
    <Phase type="Matrix" name="Fcc">
       <ParameterTable type="phase_field_general" name="">
           <Parameter type="Order_Parameter_Mobility" value="0.1" description=
""/>
           <Parameter type="Driving_Force_Scaling_Factor" value="8.0" option="
enable"

description="A factor to scale order parameter driving force"/>
           <Parameter type="Interface_Width" value="5" description="grid numbe
r of interface"/>
       </ParameterTable>
       <ParameterTable type="molar_volume" name="">
          <Parameter name="*" value="1E-5" description="Default value 1E-5"/>
       </ParameterTable>
       <ParameterTable type="stiffness_tensor" name=" description=" ">
           <Parameter name="C11" value="2.03E12" description=" "/>
```

```
            <Parameter name="C12" value="1.50e12" description=" "/>
            <Parameter name="C44" value="1.35e12" description=" "/>
      </ParameterTable>
      <Phase type="Precipitate" name="L12_Fcc">
         <ParameterTable type="inter_phase" name="" reference="Fcc">
          <Parameter type="Interfacial_Energy" value="0.025" description="J/m^
2 "/>
          <Parameter type="e11" value="-0.0005" description="Misfit strain"/>
         </ParameterTable>
      </Phase>
   </Phase>
</Alloy >
```

In this sample .pfdb file, an alloy "AlNi_Precipitation" is defined with the matrix phase "Fcc", which has a precipitate phase "L12_Fcc". More than one precipitate can be included. The precipitate name and physical properties can be defined for each precipitate phase. A set of physical parameters for each phase, such as molar volume, elastic modulus, stress-free transformation strain, interfacial energy, and so on, can be defined in "ParameterTable". Phase-field related parameter defined in the "ParameterTable" with type of "phase_field_general" are listed in Table 8.2. The physical parameters available for the precipitation model and spinodal decomposition model are listed in Table 8.3 and Table 8.4. The nucleation model related parameters are listed in Table 8.5, which are consistent with the definition in Table 5.3 of PanPrecipitaion Module.

Table 8.2 Phase-field model parameters in pfdb.

Name	**Description**
Order_Parameter_Mobility	Mobility of order parameter. This parameter decides the rate of time-evolution controlled by equation (8.10)
Driving_Force_Scaling_Factor	A scale-factor for the driving force for phase transformation. To disable it, set option to “disable”
Interface_Width	Number of grids which sample an interface between two phases. Default value is 5 grids.
Chemical_Gradient_Factor	For spinodal decomposition model only. It is used to calculate gradient energy term introduced by chemical inhomogeneous.
Chemical_Random_Amplitude	For spinodal decomposition model only. It is used to generalize initial composition profile with a sufficient degree of randomness which can initiate decomposition.
Bpq_Substract	For precipitation simulation, it decides if average elastic energy is subtracted from local elastic energy. When average elastic energy is subtracted, the overall volume fraction of precipitate phase should be independent of elastic energy. When it is set to 1, average elastic energy is subtracted from local elastic energy. Default value is 1.
Enable_Precipitate_Diffusion	For precipitation simulation, chemical mobility can be set to zero inside precipitate If matrix-diffusion is assumed to dominating the kinetics. When it is set to 1, diffusion is considered inside precipitate phases. Default value is 1.
Mean_Field_Driving_Force_Nucleation	For nucleation model, nucleation driving force can be calculated by either chemical composition or average chemical composition (mean-field) in matrix. The mean-field assumption is computationally faster. When it is set to 0, local chemical composition is used to calculate driving force of nucleation. Default is 0.

Table 8.3 Single phase physical properties in pfdb

Name	Unit	Description
molar_volume	$m^3/mole$	Molar volume of matrix or precipitate phase <ParameterTable type="molar_volume" name=""> <Parameter name="*" value="1E-5" description=""/> </ParameterTable>
stiffness_tensor	Pa	Stiffness tensor following Voigt notation. <ParameterTable type="stiffness_tensor" name="" description="Voigt notation; Orthotropic elasticity is applied when only C11, C12, C44 are set; Otherwise, set stiffness tensor explicitly"> <Parameter name="C11" value="2.03E12" description=""/> <Parameter name="C12" value="1.50e12" description=""/> <Parameter name="C44" value="1.35e12" description=""/> <!--Default values of C22 and C33 are C11--> <!--Default values of C21, C23, C32, C31 and C13 are C12--> <!--Default values of C55, C66 are C44--> <!--Default values of C45, C56 and C46 are 0.0--> <!--Default values of C14, C15, C16, C24, C25, C26, C34, C35 and C36 are 0.0--> </ParameterTable>
chemical_misfit_strain	N/A	For spinodal decomposition model only. Chemical misfit strain. <ParameterTable type="chemical_misfit_strain" name="Chemical_Misfit_Strain" reference="Fe"> <Parameter name="Ni" value="-0.01" description="Default value is 0.0"/> </ParameterTable>
mobility_scaling_factor	N/A	Scaling factor for the mobility from CALPHAD database <ParameterTable type="mobility_scaling_factor" name="Mobility_Scaling_Factor"> <Parameter name="Mo" value="6.3e-19" description="Default value is 1.0"/> </ParameterTable>

Table 8.4 Inter-phase physical properties in pfdb

Name	Unit	Description
Interfacial_Energy	J/m^2	Interfacial energy between precipitate phase and matrix phase <Parameter type="Interfacial_Energy" value="0.05" description=" "/>
e11, e12, e13, e21, e22, e23, e31, e32, e33	N/A	Stress-free transformation strain between precipitate phase and matrix phase <Parameter type="e11" value="-0.003" description=" "/> <!--Default value of e22 and e33 is e11--> <!--Default value of e12, e13, e23 is 0.0--> <!--Default value of e21 is e12--> <!--Default value of e31 is e13--> <!--Default value of e32 is e23-->

Table 8.5 Nucleation model related parameters in pfdb

Name	Unit	Description
Atomic_Spacing	*m*	Usually use lattice constant <Parameter type="Atomic_Spacing" value="7.6E10" description="Atomic Spacing" />
Nucleation_Site_Parameter	N/A	Homogenous model only for the pre-installed precipitation model
Steady_State_Nucleation_Rate	N/A	Set to 1 if steady state nucleation rete is applied. <Parameter type="Steady_State_Nucleation_Rate" value="1" description="Indicate if steady state nucleation rate is applied" />
Driving_Force_Factor	N/A	A scaling factor of nucleation driving force
Effective_Diffusivity_Factor	N/A	A scaling factor of effective diffusivity for nucleation rate model
Shield_Time	Second	A time period in which stability of nuclei is numerically sustained.

8.4 Tutorial

8.4.1 Step 1: Create a PanPhaseField Project

One can create a PanPhaseFieldproject through menu "**File → Create a New Workspace**" or "**File → Add a New Project**" in an existing workspace. The "Module Window" pops out for user to choose a module for the new project as shown in Figure 8.3. Choose "PanPhaseField" module for phase-field simulation, and the PanPhaseField project will be created after user click on **Create** button or double click on the PanPhaseField icon.

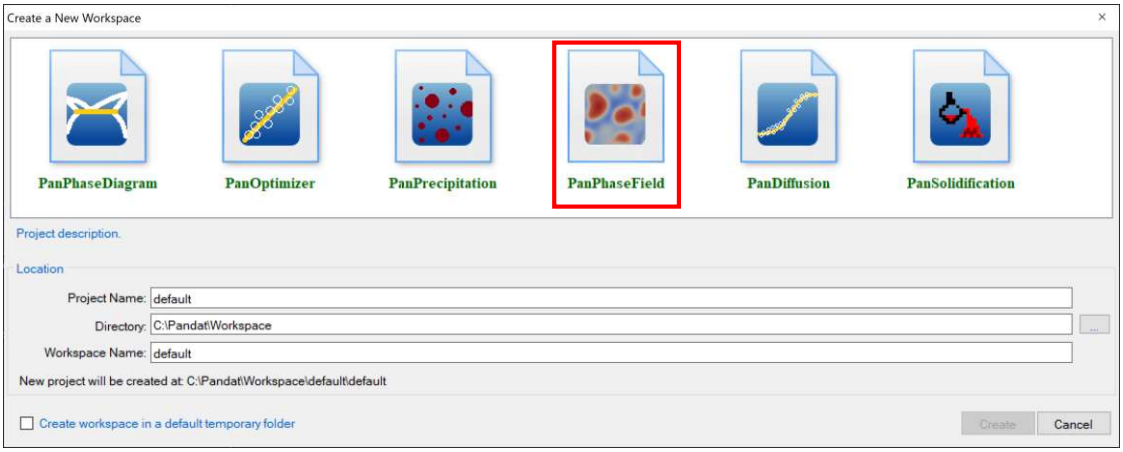

Figure 8.3 Creating a PanPhaseField workspace