**Figure Captions**

Fig. 1 The orthorhombic (A17) structure (a) in a perspective view and (b) in a projection on xy plane and the rhombohedral (A7) structure (c) in a perspective view and (d) in a projection along x+y+z direction. In the projections, P atoms in the lower layer are designated using a filled circle [16].

Fig. 2 Pressure dependence of atomic volume of transformed structures of black phosphorus, (a) simple cubic, (b) simple hexagonal and (c) bcc phase calculated using the present 2NN MEAM potential, in comparison with experimental data [40,41,43].

Fig. 3 Enthalpy of mixing of the Fe-P liquid alloys calculated using the present 2NN MEAM potential, in comparison with experimental data [68].

Fig. 4 Illustration of a substitutional (Psubs) P atom, octahedral, tetrahedral interstitial P atom, and mixed dumbbells, <110>Fe-P and <111>Fe-P. The small black spheres and large white spheres represent P and Fe atoms, respectively.

Fig. 5 The relationship between the chemical potential difference () and bulk  
concentration of phosphorus at various temperatures, calculated using the present

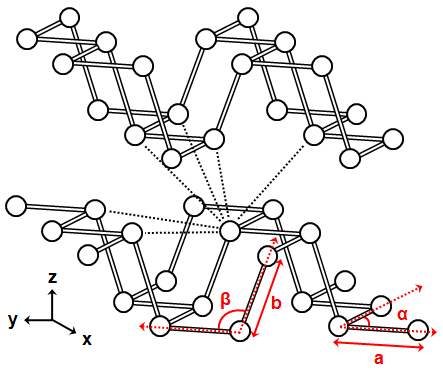
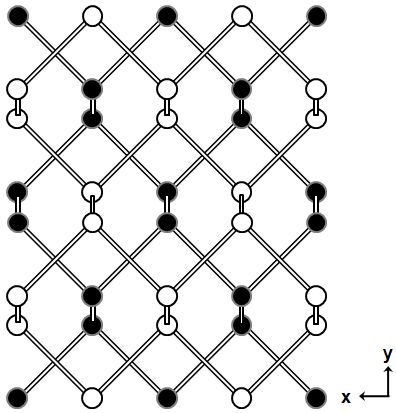
2NN MEAM potential.

Fig. 6 Schematic illustration of simulation samples for twist GBs in bcc Fe. The axis of rotation, [100] for high angle and low angle incoherent GBs, and [110] for the special (Σ3) GB, are parallel to the y-direction.

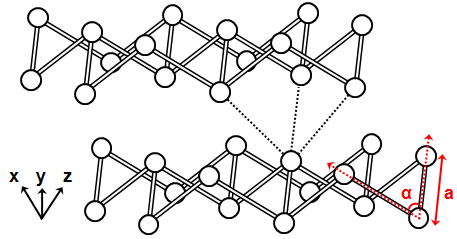
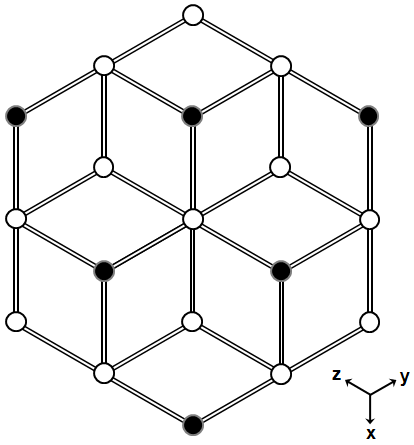
Fig. 7 Distribution of P atoms on GBs of bcc Fe-0.1 at% P alloys at 900 K, calculated using the present 2NN MEAM potential. Front view on the normal direction of the (a) high angle (Σ241), (b) low angle (Σ257), and (c) special GB (Σ3) planes and lateral view of the (d) high angle, (e) low angle, and (f) special GB planes. Gray spheres represent Fe atoms and black (dark brown) spheres represent P atoms.

Fig. 8 Concentration profiles of P atoms on the (a) high angle, (b) low angle, and (c) special GBs for the 0.1 at% bulk concentration of P at temperatures between 600 and 1300 K with Gaussian fitting (solid lines), calculated using the present 2NN MEAM potential, and (d) the definition of GB thickness.

Fig. 9 GB concentration of P atoms (a) vs. bulk concentration of P at 900 K and (b) vs. temperature for the 0.1 at% bulk concentration of P, calculated using the present 2NN MEAM potential.

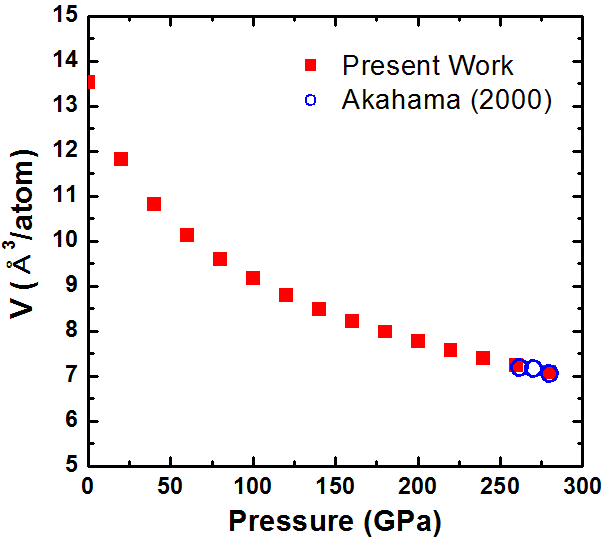
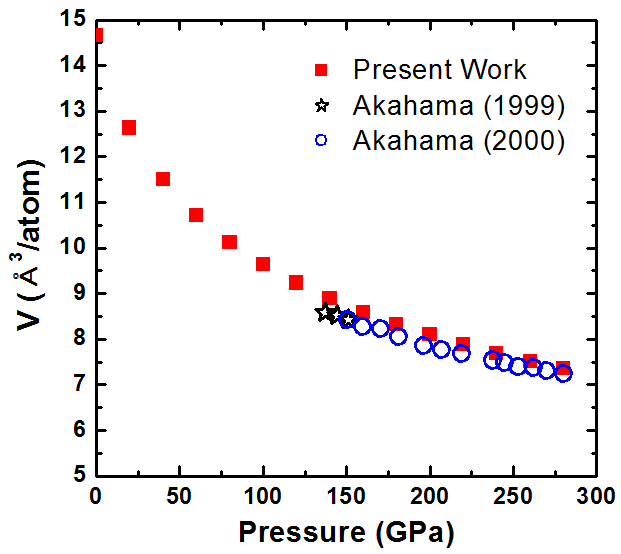
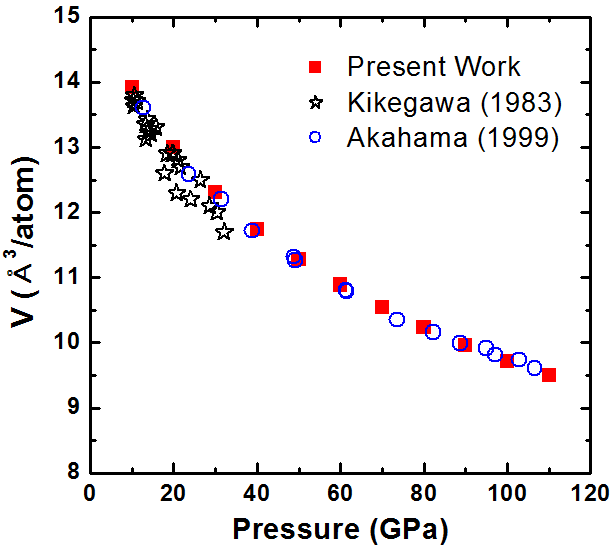
 

**(a) (b)**

**(c) (d)**

Fig. 1 The orthorhombic (A17) structure (a) in a perspective view and (b) in a projection on xy plane and the rhombohedral (A7) structure (c) in a perspective view and (d) in a projection along x+y+z direction. In the projections, P atoms in the lower layer are designated using a filled circle [16].



**(a) (b) (c)**

Fig. 2 Pressure dependence of atomic volume of transformed structures of black phosphorus, (a) simple cubic, (b) simple hexagonal and (c) bcc phase calculated using the present 2NN MEAM potential, in comparison with experimental data [40,41,43].

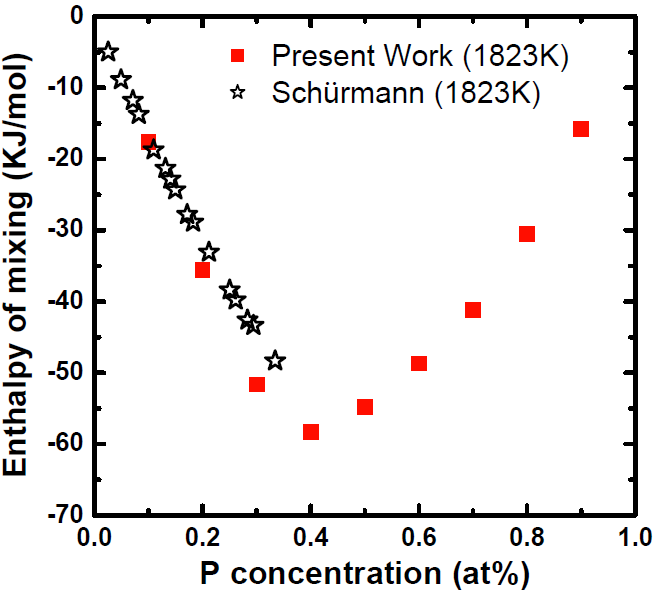


Fig. 3 Enthalpy of mixing of the Fe-P liquid alloys calculated using the present 2NN MEAM potential, in comparison with experimental data [68].

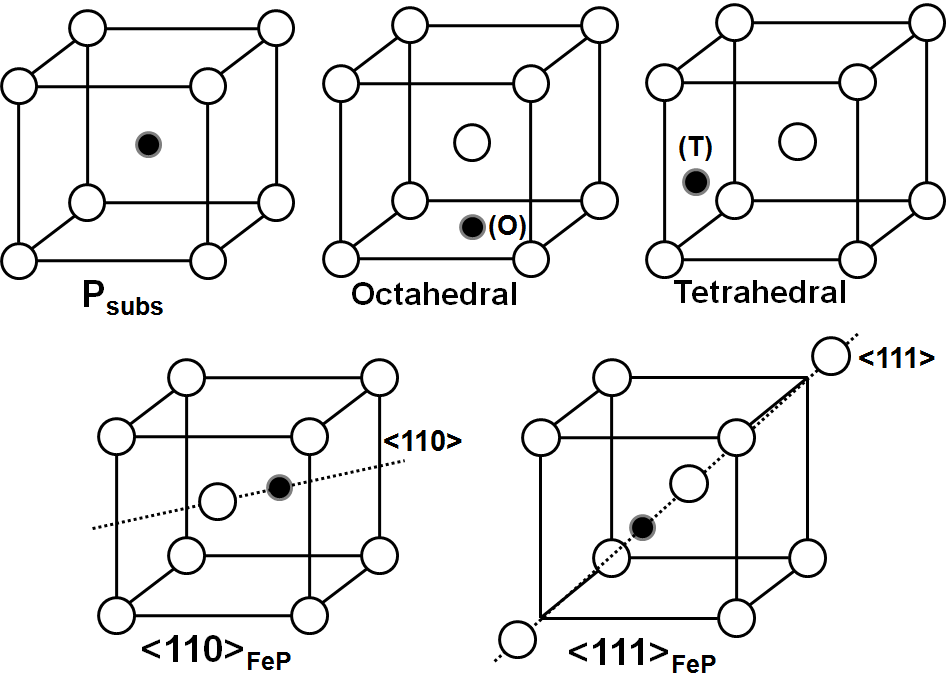


Fig. 4 Illustration of a substitutional (Psubs) P atom, octahedral, tetrahedral interstitial P atom, and mixed dumbbells, <110>Fe-P and <111>Fe-P. The small black spheres and large white spheres represent P and Fe atoms, respectively.

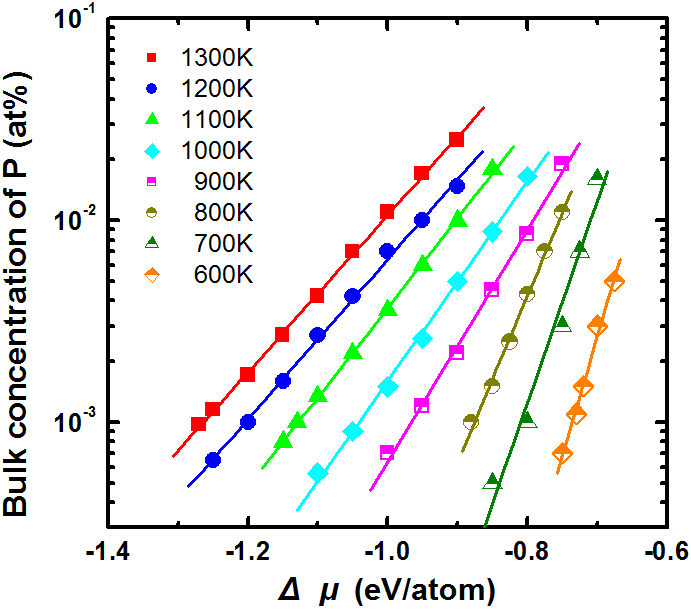


Fig. 5 The relationship between the chemical potential difference () and bulk  
concentration of phosphorus at various temperatures, calculated using the present

2NN MEAM potential.

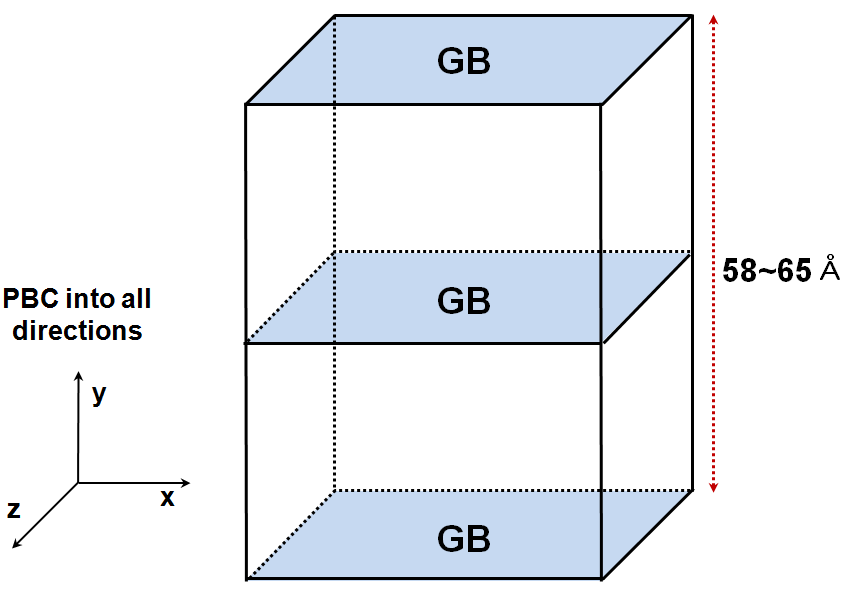
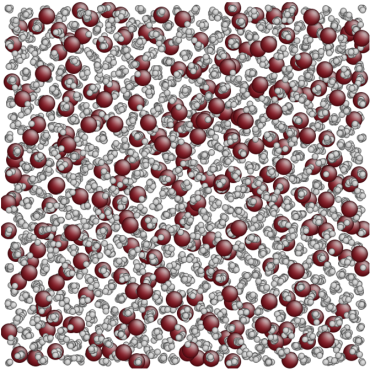
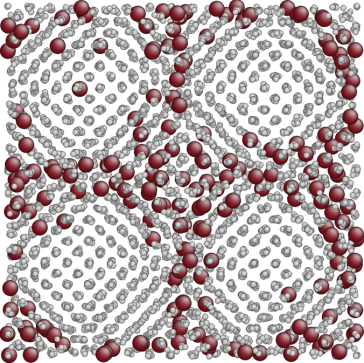
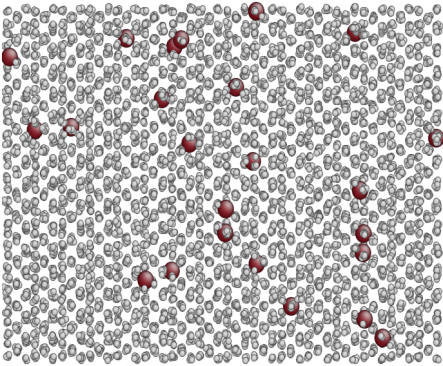
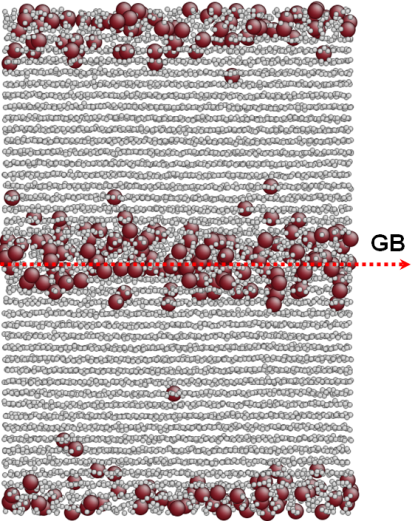
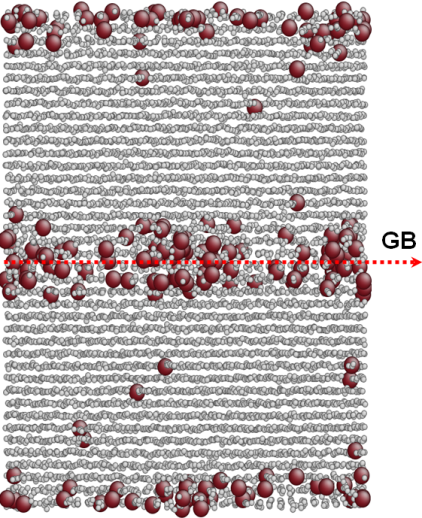
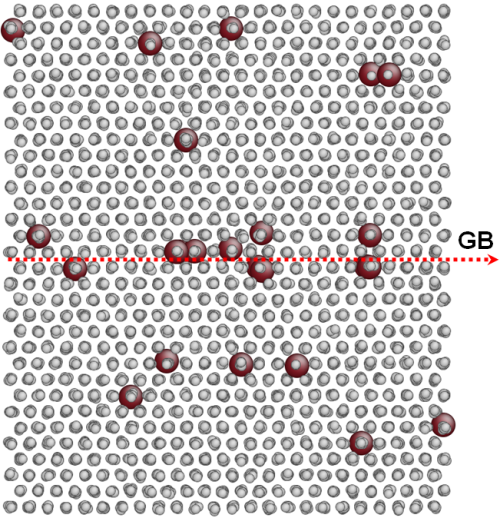


Fig. 6 Schematic illustration of simulation samples for twist GBs in bcc Fe. The axis of rotation, [100] for high angle and low angle incoherent GBs, and [110] for the special (Σ3) GB, are parallel to the y-direction.

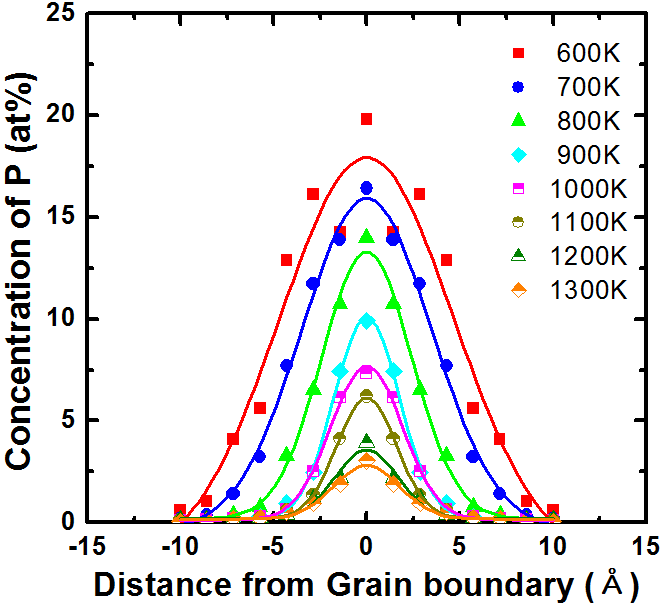
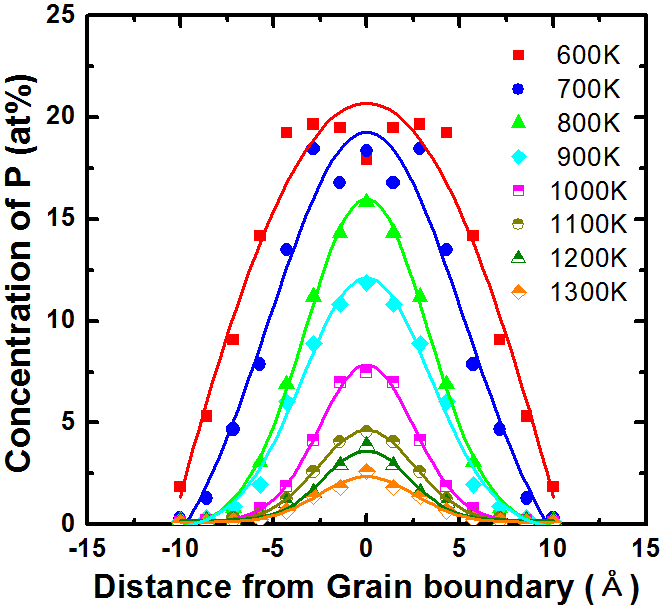
  

**(a) (b) (c)**

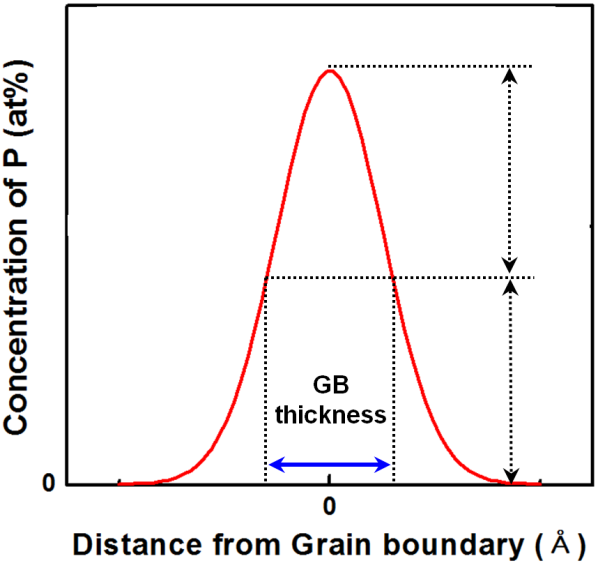
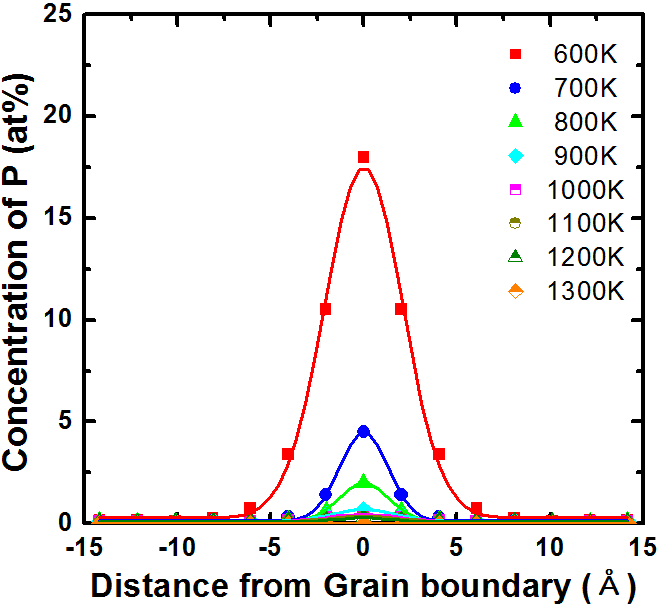
  

**(d) (e) (f)**

Fig. 7 Distribution of P atoms on GBs of bcc Fe-0.1 at% P alloys at 900 K, calculated using the present 2NN MEAM potential. Front view on the normal direction of the (a) high angle (Σ241), (b) low angle (Σ257), and (c) special GB (Σ3) planes and lateral view of the (d) high angle, (e) low angle, and (f) special GB planes. Gray spheres represent Fe atoms and black (dark brown) spheres represent P atoms.

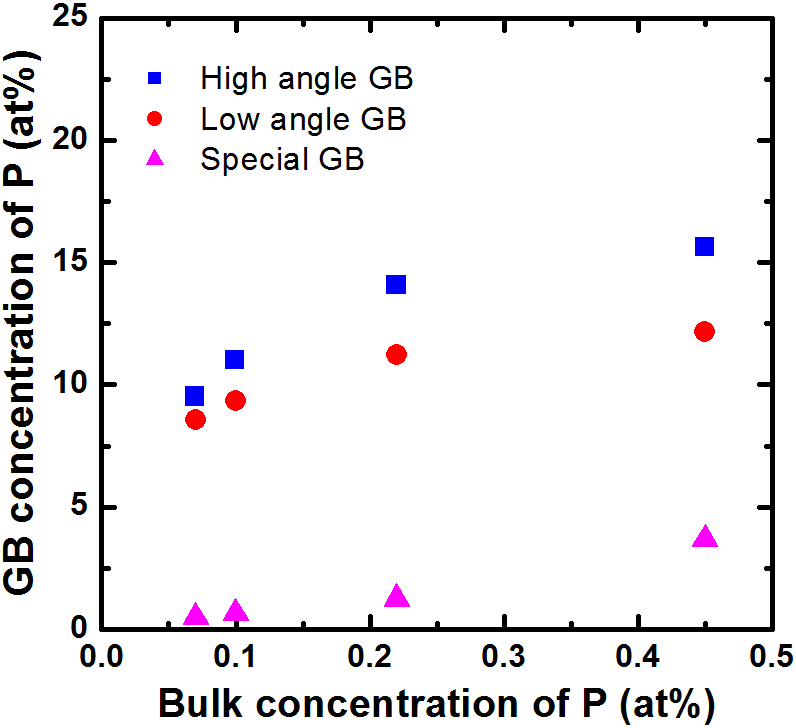
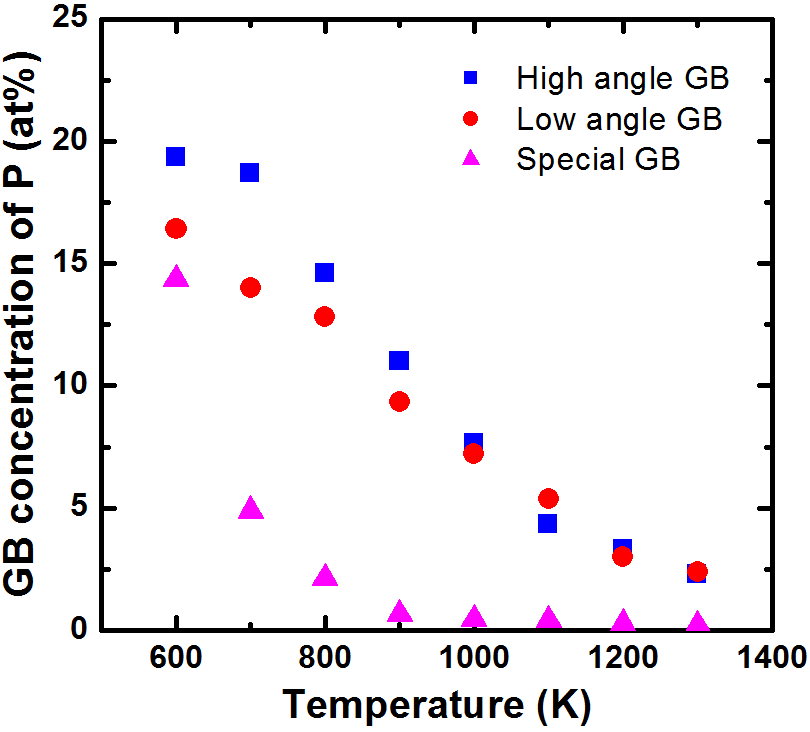


**(a) (b)**



**(c) (d)**

Fig. 8 Concentration profiles of P atoms on the (a) high angle, (b) low angle, and (c) special GBs for the 0.1 at% bulk concentration of P at temperatures between 600 and 1300 K with Gaussian fitting (solid lines), calculated using the present 2NN MEAM potential, and (d) the definition of GB thickness.

**(a) (b)**

Fig. 9 GB concentration of P atoms (a) vs. bulk concentration of P at 900 K and (b) vs. temperature for the 0.1 at% bulk concentration of P, calculated using the present 2NN MEAM potential.