Formation and models of Mg_2Si seed layers on Si with (111), (100), and (110) orientations for Ca_2Si sacrificial epitaxy

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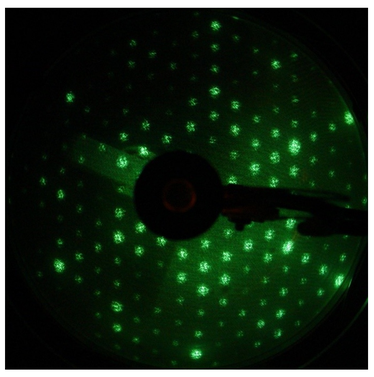
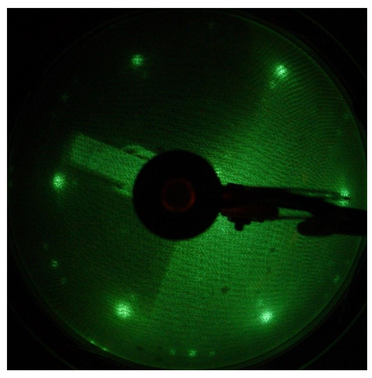
Mg_2Si on Si(111)

Clean sample



surface reconstruction Si(111)7×7

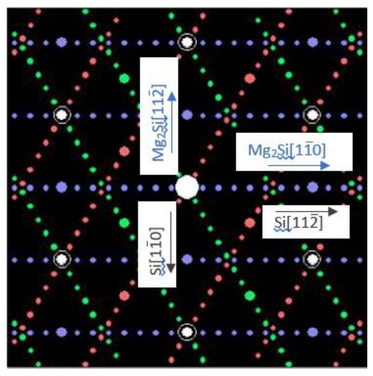
Mg on Si(111) at 150 °C



surface reconstruction Mg_2Si(111)"1×8"

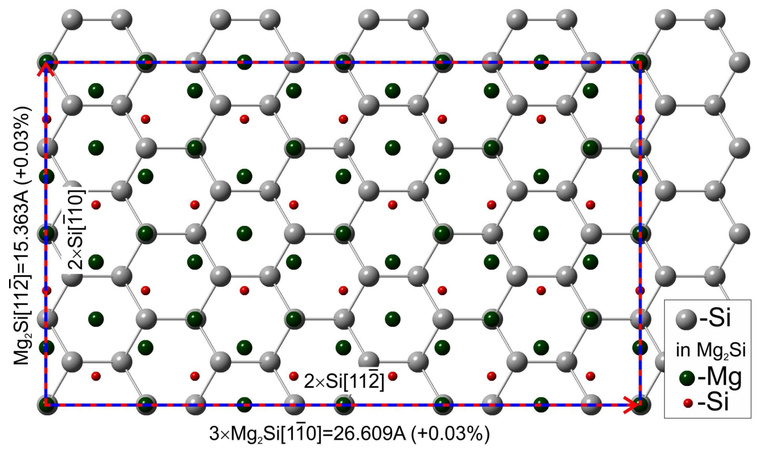
Epitaxial relations:
$Mg_2Si(111)||Si(111)$
$Mg_2Si[11\text{-}2]||Si[\text{-}110]$
$Mg_2Si[1\text{-}10]||Si[11\text{-}2]$

LEED modeling

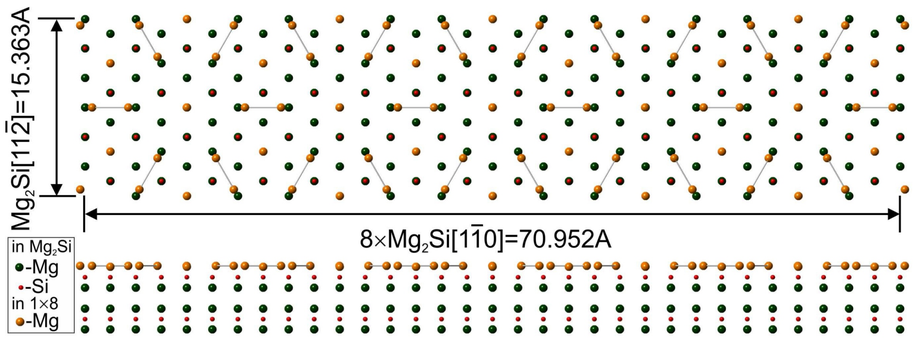


surface reconstruction Mg_2Si(111)"1×8" on Si(111) surface

Model of Mg_2Si(111) on Si(111)



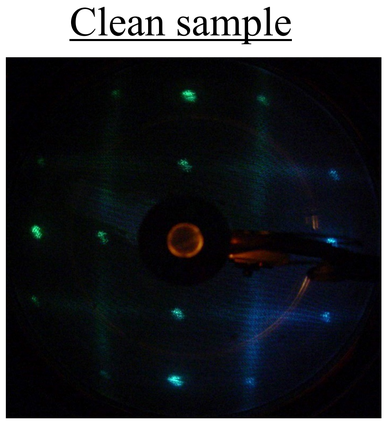
Model of surface reconstruction Mg_2Si(111)"1×8"



Lattice constants: Mg_2Si a=6.2718 Å (-1.9%), Si a=5.43 Å.

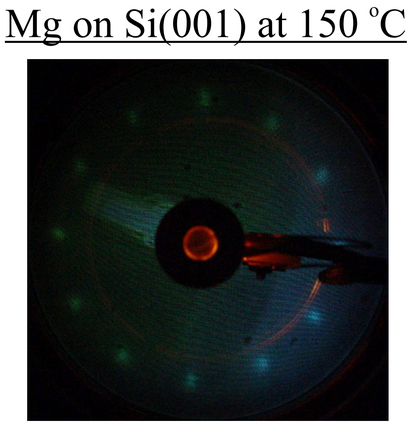
Mg_2Si on Si(001)

Clean sample



surface reconstruction Si(001)2×1

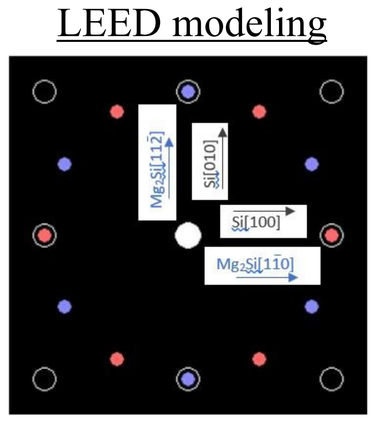
Mg on Si(001) at 150 °C



surface reconstruction Mg_2Si(111)1×1

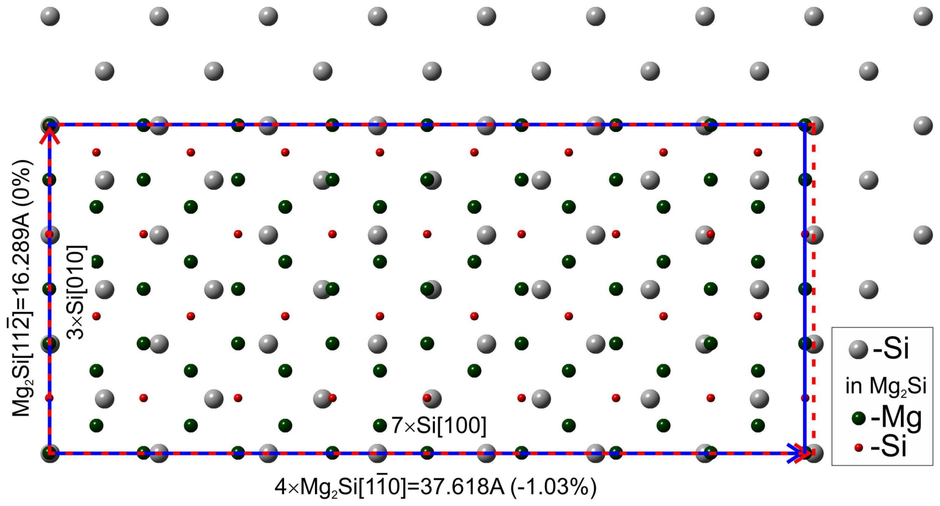
Epitaxial relations:
$Mg_2Si(111)||Si(001)$
$Mg_2Si[11\text{-}2]||Si[010]$
$Mg_2Si[1\text{-}10]||Si[100]$

LEED modeling



surface reconstruction Mg_2Si(111)1×1 on Si(001) surface

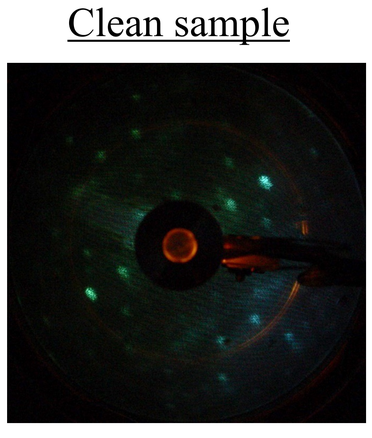
Model of Mg_2Si(111) on Si(001)



Lattice constants: Mg_2Si a=6.65 Å (4.05%), Si a=5.43 Å.

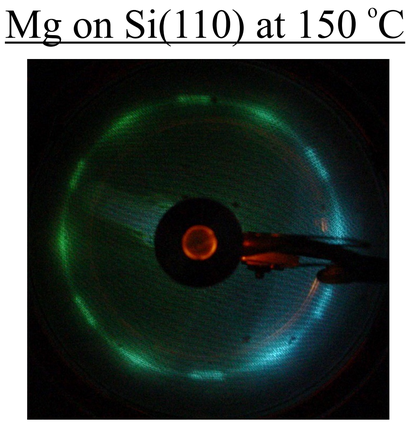
Mg_2Si on Si(110)

Clean sample



surface reconstruction Si(110)"16×2"

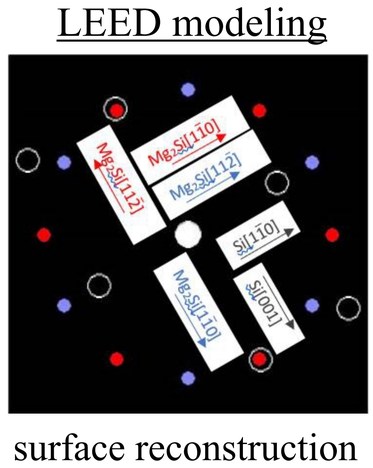
Mg on Si(110) at 150 °C



surface reconstruction Mg_2Si(111)1×1

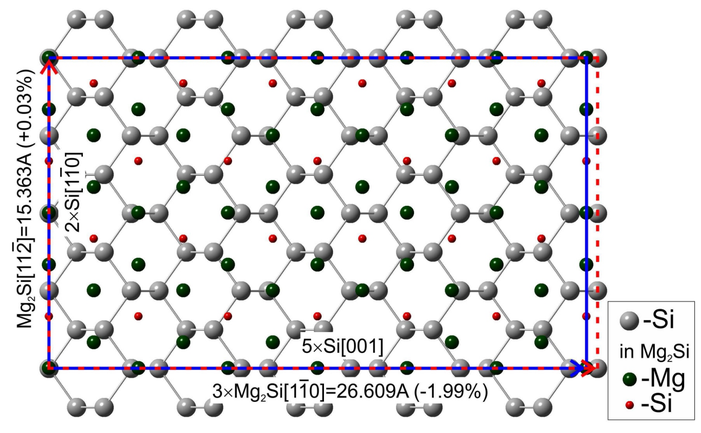
Epitaxial relations:
$Mg_2Si(111)||Si(001)$
$Mg_2Si[11\text{-}2]||Si[010]$
$Mg_2Si[1\text{-}10]||Si[100]$

LEED modeling



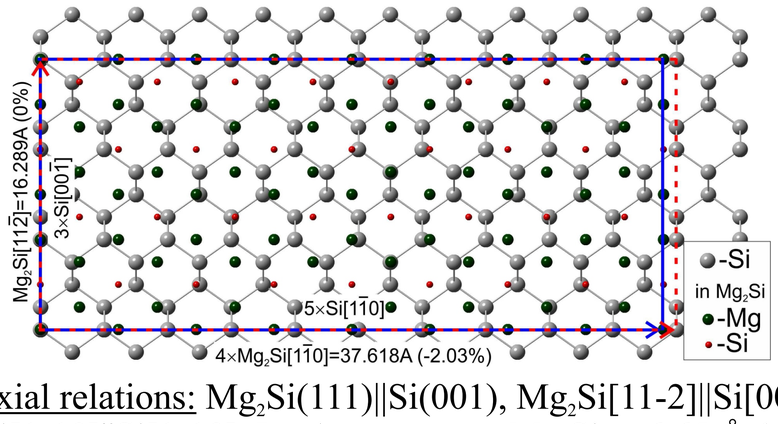
surface reconstruction Mg_2Si(111)1×1 on Si(110) surface

Model of 1st type NC Mg_2Si(111) on Si(110)



Epitaxial relations: $Mg_2Si(111)||Si(001)$, $Mg_2Si[11\text{-}2]||Si[1\text{-}10]$, $Mg_2Si[1\text{-}10]||Si[001]$. Lattice constant: Mg_2Si a=6.2718 Å (-1.9%).

Model of 2nd type NC Mg_2Si(111) on Si(110)



Epitaxial relations: $Mg_2Si(111)||Si(001)$, $Mg_2Si[11\text{-}2]||Si[00\text{-}1]$, $Mg_2Si[1\text{-}10]||Si[1\text{-}10]$. Lattice constant: Mg_2Si a=6.65 Å (4.05%).

Conclusions

1. Mg_2Si film grows epitaxially on Si(111), Si(001), and Si(110).
2. Formation of surface reconstruction Mg_2Si(111)"1×8" takes place during Mg_2Si film growth on Si(111).
3. Mg_2Si better matches its lattice on the Si(111) surface, while worse on the Si(110) surface.