Modulus Spaces

Calculations for Young's modulus in the various crystallographic orientations for several cubic elements.

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Define the appropriate equations.

Define the components of the unit direction vector as functions of θ and ϕ.

```
xu[θ_, ϕ_] := Cos[θ] Cos[ϕ]
yu[θ_, ϕ_] := Sin[θ] Cos[ϕ]
zu[θ_, ϕ_] := Sin[ϕ]
```

Define the direction cosines as functions of θ and ϕ.

```
α[θ_, ϕ_] := {1, 0, 0}.{xu[θ, ϕ], yu[θ, ϕ], zu[θ, ϕ]}
β[θ_, ϕ_] := {0, 1, 0}.{xu[θ, ϕ], yu[θ, ϕ], zu[θ, ϕ]}
γ[θ_, ϕ_] := {0, 0, 1}.{xu[θ, ϕ], yu[θ, ϕ], zu[θ, ϕ]}
```

Define the elastic modulus in direction <hkl> as functions of θ and ϕ.

ehkl[θ_, ϕ_] :=

$$\left(\frac{1}{\text{e100}} - 3\left(\frac{1}{\text{e100}} - \frac{1}{\text{e111}}\right)\left(\alpha[\theta, \phi]^2 \beta[\theta, \phi]^2 + \alpha[\theta, \phi]^2 \gamma[\theta, \phi]^2 + \beta[\theta, \phi]^2 \gamma[\theta, \phi]^2\right)\right)^{-1}$$

Define the elastic modulus in direction <hkl> as functions of direction cosines a, b, and g.

$$\text{eabg[a\_, b\_, g\_] :=} \left(\frac{1}{\text{e100}} - 3\left(\frac{1}{\text{e100}} - \frac{1}{\text{e111}}\right)\left(a^2 b^2 + a^2 g^2 + b^2 g^2\right)\right)^{-1}$$

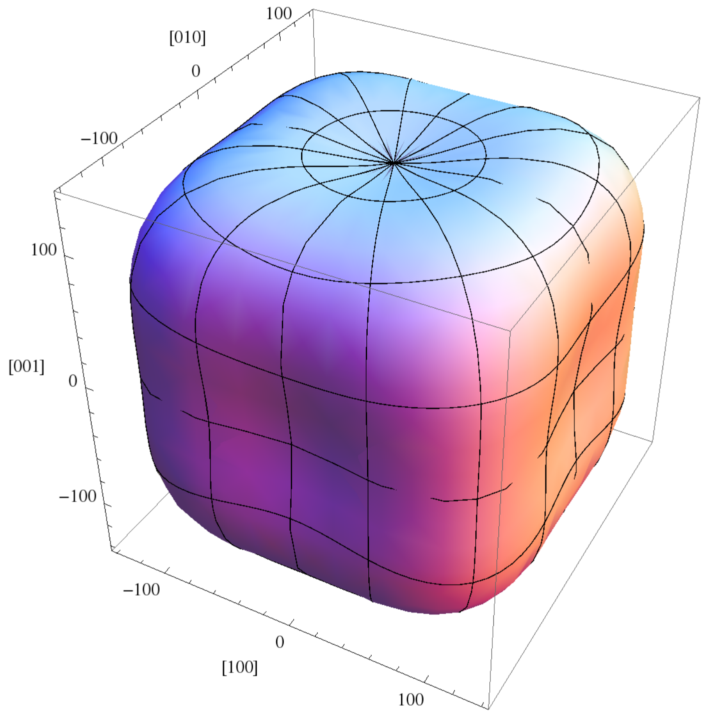
Calculations for Si

Define the moduli for Si in GPa.

```
e100 = 130;
e111 = 189;
```

Plot the modulus surfuce for Si.

```
ParametricPlot3D[{ehkl[θ, ϕ] xu[θ, ϕ], ehkl[θ, ϕ] yu[θ, ϕ], ehkl[θ, ϕ] zu[θ, ϕ]},
 {θ, 0, 2 π}, {ϕ, -π, π}, AxesLabel → {"[100]", "[010]", "[001]"}]
```



Look at the modulus within the (111) plane

Define new coordinate system (unit vector directions) with z' along <111> direction and x' and y' in (111) plane. Define parameter t as angle from x' axis for unit vector v as function of t in the x'-y' plane, i.e. (111) plane. Define functions to calculate the direction cosines of vector v as functions of t.

$$xp = \frac{1}{\sqrt{6}} \{2, -1, -1\};$$

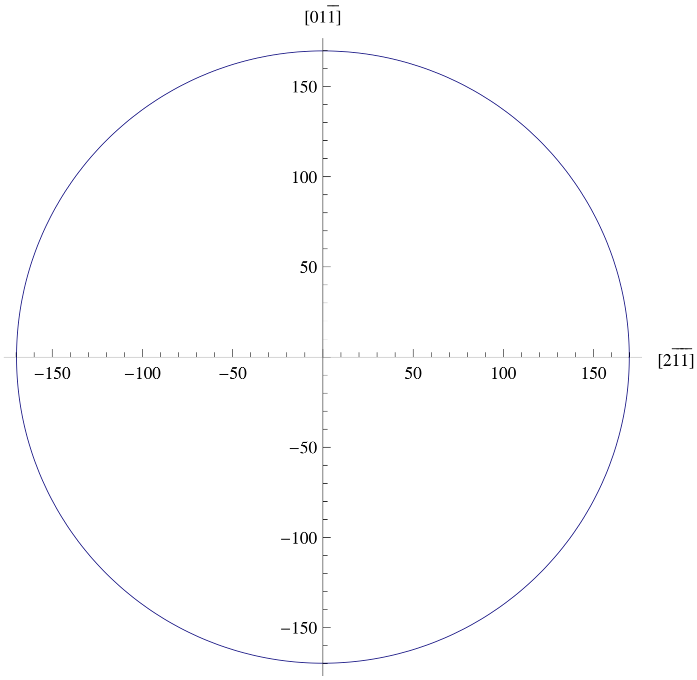
$$yp = \frac{1}{\sqrt{2}} \{0, 1, -1\};$$

$$zp = \frac{1}{\sqrt{3}} \{1, 1, 1\};$$

```
v[t_] := xp Cos[t] + yp Sin[t]
alpha[t_] := v[t].{1, 0, 0}
beta[t_] := v[t].{0, 1, 0}
gamma[t_] := v[t].{0, 0, 1}
```

Plot the modulus of Si in the (111) plane.

```
ParametricPlot[{eabg[alpha[t], beta[t], gamma[t]] Cos[t],
  eabg[alpha[t], beta[t], gamma[t]] Sin[t]},
 {t, 0, 2 π}, AspectRatio → 1, AxesLabel → {"[2-1-1]", "[01-1]"}]
```



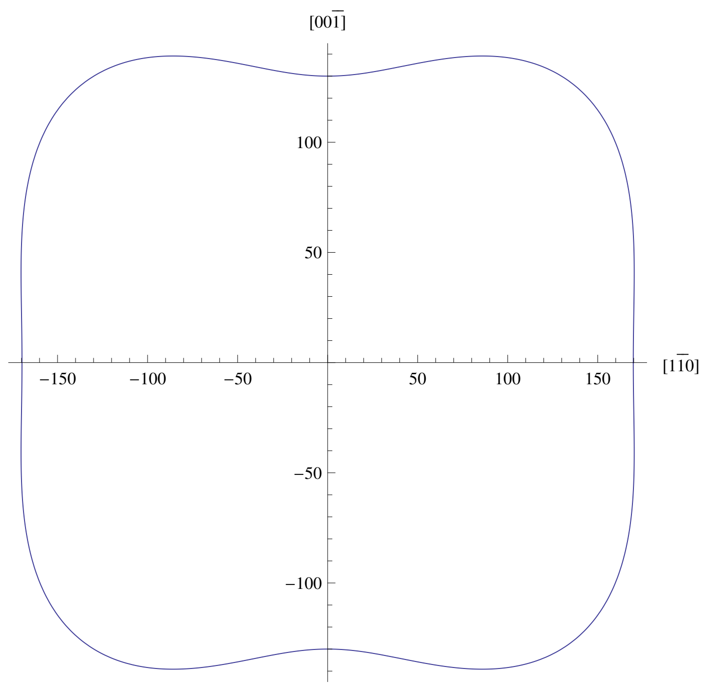
Look at the modulus within the (110) plane

Define new coordinate system (unit vector directions) with z' along <110> direction and x' and y' in (110) plane. Define parameter t as angle from x' axis for unit vector v as function of t in the x'-y' plane, i.e. (110) plane. Define functions to calculate the direction cosines of vector v as functions of t.

```
xp = 1/Sqrt[2] {1, -1, 0};
yp = {0, 0, -1};
zp = 1/Sqrt[2] {1, 1, 0};
v[t_] := xp Cos[t] + yp Sin[t]
alpha[t_] := v[t].{1, 0, 0}
beta[t_] := v[t].{0, 1, 0}
gamma[t_] := v[t].{0, 0, 1}
```

Plot the modulus of Si in the (110) plane.

```
ParametricPlot[{eabg[alpha[t], beta[t], gamma[t]] Cos[t],
  eabg[alpha[t], beta[t], gamma[t]] Sin[t]},
 {t, 0, 2 π}, AspectRatio → 1, AxesLabel → {"[11̄0]", "[001̄]"}]
```



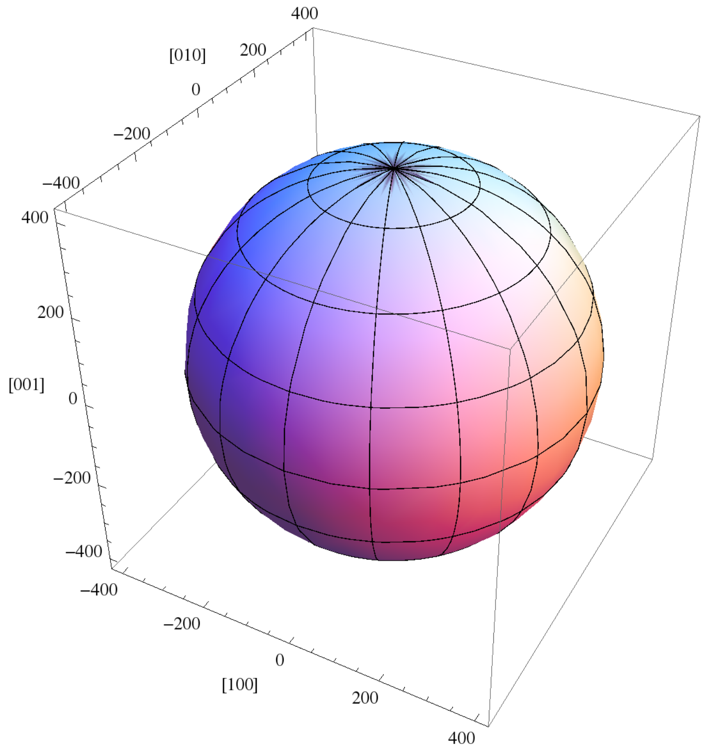
Calculations for W

Define the moduli for W in GPa.

```
e100 = 411;
e111 = 411;
```

Plot the modulus surface for W. Note that it is spherical!

```
ParametricPlot3D[{ehkl[θ, ϕ] xu[θ, ϕ], ehkl[θ, ϕ] yu[θ, ϕ], ehkl[θ, ϕ] zu[θ, ϕ]},
 {θ, 0, 2 π}, {ϕ, -π, π}, AxesLabel → {"[100]", "[010]", "[001]"}]
```



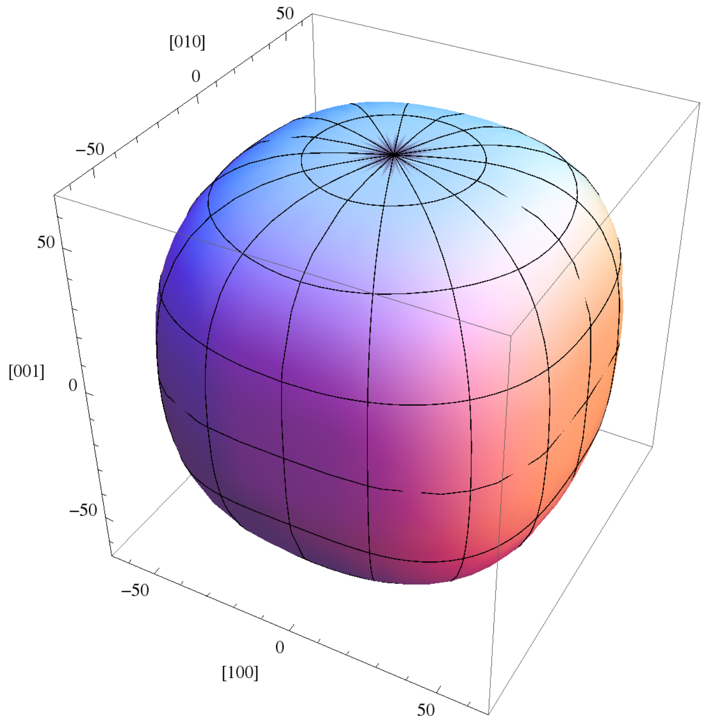
Calculations for Al

Define the moduli for Al in GPa.

```
e100 = 64;
e111 = 76;
```

Plot the modulus surface for Al.

```
ParametricPlot3D[{ehkl[θ, ϕ] xu[θ, ϕ], ehkl[θ, ϕ] yu[θ, ϕ], ehkl[θ, ϕ] zu[θ, ϕ]},
 {θ, 0, 2 π}, {ϕ, -π, π}, AxesLabel → {"[100]", "[010]", "[001]"}]
```



Calculations for Fe

Define the moduli for Fe in GPa.

```
e100 = 129;
e111 = 276;
```

Plot the modulus surface for Fe.

```
ParametricPlot3D[{ehkl[θ, ϕ] xu[θ, ϕ], ehkl[θ, ϕ] yu[θ, ϕ], ehkl[θ, ϕ] zu[θ, ϕ]},
 {θ, 0, 2 π}, {ϕ, -π, π}, AxesLabel → {"[100]", "[010]", "[001]"}]
```