

Miller - Bravais or Weber indices

1. Transforming [uvw] indices to Weber [uvtw] indices

Miller-Bravais (Weber for the Swiss) indices [uvtw] have been defined in order to obtain all equivalent crystal directions by permutating the [uvw] triplets. This is achieved by the Weber matrix defined as:

```
In[1]:= toWeberTransform = {{2, -1, 0}, {-1, 2, 0}, {-1, -1, 0}, {0, 0, 3}}
toWeberTransform // MatrixForm
```

```
Out[1]:= {{2, -1, 0}, {-1, 2, 0}, {-1, -1, 0}, {0, 0, 3}}
```

```
Out[2]/MatrixForm=
```

$$\begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & 0 \\ -1 & -1 & 0 \\ 0 & 0 & 3 \end{pmatrix}$$

A list of [uvw] :

```
In[3]:= uvw = {{1, 0, 0}, {1, 1, 0}, {0, 0, 1}, {2, 1, 0}, {1, 0, 1},
          {1, 1, 1}, {2, 1, 1}, {2, 0, 1}, {2, 2, 1}, {3, 1, 0}, {3, 2, 0}}
```

```
Out[3]:= {{1, 0, 0}, {1, 1, 0}, {0, 0, 1}, {2, 1, 0}, {1, 0, 1},
          {1, 1, 1}, {2, 1, 1}, {2, 0, 1}, {2, 2, 1}, {3, 1, 0}, {3, 2, 0}}
```

indices is transformed to [uvtw] ones by :

```
In[4]:= uvtw = (toWeberTransform . #) & /@ uvw
```

```
Out[4]:= {{2, -1, -1, 0}, {1, 1, -2, 0}, {0, 0, 0, 3}, {3, 0, -3, 0}, {2, -1, -1, 3}, {1, 1, -2, 3},
          {3, 0, -3, 3}, {4, -2, -2, 3}, {2, 2, -4, 3}, {5, -1, -4, 0}, {4, 1, -5, 0}}
```

And then simplified:

```
In[5]:= (# / GCD @@ #) & /@ uvtw
```

```
Out[5]:= {{2, -1, -1, 0}, {1, 1, -2, 0}, {0, 0, 0, 1}, {1, 0, -1, 0}, {2, -1, -1, 3}, {1, 1, -2, 3},
          {1, 0, -1, 1}, {4, -2, -2, 3}, {2, 2, -4, 3}, {5, -1, -4, 0}, {4, 1, -5, 0}}
```

Using a (very) simple Module[] :

```
In[6]:= toWeber [uvw_List] :=
Module [{toWeberTransform = {{2, -1, 0}, {-1, 2, 0}, {-1, -1, 0}, {0, 0, 3}}, uvtw},
  uvtw = toWeberTransform . uvw;
  uvtw / GCD @@ uvtw]
```

```
In[7]:= toWeber [#] & /@ uvw
```

```
Out[7]:= {{2, -1, -1, 0}, {1, 1, -2, 0}, {0, 0, 0, 1}, {1, 0, -1, 0}, {2, -1, -1, 3}, {1, 1, -2, 3},
          {1, 0, -1, 1}, {4, -2, -2, 3}, {2, 2, -4, 3}, {5, -1, -4, 0}, {4, 1, -5, 0}}
```

```
In[8]:= Print [#,"->", toWeber [#]] & /@ uvw;
```

```
{1, 0, 0}->{2, -1, -1, 0}
{1, 1, 0}->{1, 1, -2, 0}
{0, 0, 1}->{0, 0, 0, 1}
{2, 1, 0}->{1, 0, -1, 0}
{1, 0, 1}->{2, -1, -1, 3}
{1, 1, 1}->{1, 1, -2, 3}
{2, 1, 1}->{1, 0, -1, 1}
{2, 0, 1}->{4, -2, -2, 3}
{2, 2, 1}->{2, 2, -4, 3}
{3, 1, 0}->{5, -1, -4, 0}
{3, 2, 0}->{4, 1, -5, 0}
```

It is readily apparent that all hexagonal directions equivalent to [1,0,0] will be given by the permutation of:

```
In[9]:= toWeber[{1, 0, 0}]
```

```
Out[9]:= {2, -1, -1, 0}
```

This is verified for [1, 1, 0], [-1,1,0], ...

```
In[10]:= {toWeber[{1, 1, 0}], toWeber[{0, 1, 0}]}
```

```
Out[10]:= {{1, 1, -2, 0}, {-1, 2, -1, 0}}
```

2. Transforming [uvtw] Weber indices to common [uvw] indices

The transform from Weber [uvtw] to common [uvw] is defined by :

```
In[11]:= fromWeberTransform = {{2/3, 1/3, 0, 0}, {1/3, 2/3, 0, 0}, {0, 0, 0, 1/3}};
fromWeberTransform // MatrixForm
```

```
Out[12]/MatrixForm=
```

$$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0 & 0 \\ \frac{1}{3} & \frac{2}{3} & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{3} \end{pmatrix}$$

```
In[13]:= uvw = (fromWeberTransform . #) & /@ uvtw
```

```
Out[13]:= {{1, 0, 0}, {1, 1, 0}, {0, 0, 1}, {2, 1, 0}, {1, 0, 1},
{1, 1, 1}, {2, 1, 1}, {2, 0, 1}, {2, 2, 1}, {3, 1, 0}, {3, 2, 0}}
```

In[29]=

```

fromWeber [uvtw_List] := Module [ {denominator =
    fromWeberTransform = { { {2, 1, 0, 0}, {1, 2, 0, 0}, {0, 0, 0, 1} }, uvw },
    uvw = fromWeberTransform . uvtw;
    denominator = Times @@ (Denominator [#] & /@ uvw);
    uvw = denominator uvw;
    uvw / GCD @@ uvw ]

```

3. Verifying the transforms

A list of [uvw] is generated :

In[43]=

```

uvw = Table [ {i, j, k}, {i, 10}, {j, 10}, {k, 10} // Flatten [# , 2] &;
uvw = (# / GCD @@ #) & /@ uvw;
uvw = Union [uvw]

```

Out[45]=

```

{ {1, 1, 1}, {1, 1, 2}, {1, 1, 3}, {1, 1, 4}, {1, 1, 5}, {1, 1, 6}, {1, 1, 7}, {1, 1, 8},
  {1, 1, 9}, {1, 1, 10}, {1, 2, 1}, {1, 2, 2}, {1, 2, 3}, {1, 2, 4}, {1, 2, 5}, {1, 2, 6},
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The [uvw] are transformed to Weber [uvtw] :

In[46]=

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uvw = toWeber [#] & /@ uvw
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Out[46]=

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{19, -8, -11, 21}, {19, -8, -11, 24}, {19, -8, -11, 27}, {19, -8, -11, 30},
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```

In[49]=

```
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Out[49]=

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```

The back transformed [uvw] indices are compared to the initial [uvw] :

In[50]:=

```
uvwBack == uvw
```

Out[50]=

```
True
```

4. Note

A **very common error** is to assume that it suffices to let $t = -(u + v)$ to get proper Miller-Bravais (or Weber) indices. This is wrong! It is only valid for (h k l) plane indices, i.e. (h k l) \rightarrow (h k $-(h+k)$ l). Have a look in help documentation of jems stereographic projection or help/WeberIndices.htm!