for lune separation is distinct from the requirement for spot separation. If lunes overlap, spots may have more than one index consistent with a particular position on the detector.

The autoindexing procedure described above is not dependent on prior knowledge of the crystal unit cell; however, for efficiency reasons, the search is restricted to a reasonable range of unit-cell dimensions, obtained, for example, from the requirement of spot separation. In *DENZO*, this default can be overridden by the keyword 'longest vector', but the need to use this keyword is a sign of a problem that should be fixed. Either the defined spot size should be decreased or data should be recollected with the detector further away from the crystal.

11.4.3.4. *Misindexing*

Autoindexing is sensitive to inaccuracy in the description of the detector geometry. The specified position of the beam on the detector should correspond to the origin of the Bragg-peaks lattice (Miller index 000). Autoindexing will shift the origin of the lattice to the nearest Bragg lattice point. An incorrect beam position will result in the nearest Bragg lattice point not having the index 000. In such a situation, all reflections will have incorrectly determined indices. Such misindexing can be totally self-consistent until the intensities of symmetry-related reflections are compared. This dependence of the indexing correctness on the assumed beam position is the main source of difficulties in indexing (Gewirth, 1996; Otwinowski & Minor, 1997). The beam position has to be precise, as the largest acceptable error is one half of the shortest distance between spots.

Indexing limited to determining h, k, l triplets is not very sensitive to other detector parameters. Errors by a degree or two in rotation or by 10% in distance are unlikely to produce wrong values of h, k and l. Sometimes even a very large error, such as the distance being too large by a factor of 5, will still produce the correct h, k, l triplets. The detector position error will be compensated by an error in the lattice determined by autoindexing. For this reason, the accuracy of the lattice is not a function of the autoindexing procedure, but depends mainly on the accuracy of the detector description. By the same token, the distortion of the lattice also depends on the accuracy of the detector parameters.

11.4.3.5. *Twins*

Special care has to be taken if more than one crystal contributes to the diffraction image. When there is a large disproportion between volumes (*e.g.* the presence of a satellite crystal), autoindexing may work without any modifications. In the case of similar volumes, the manual editing of weaker reflections and resolution cuts can make the proportion of reflections from one crystal in the peak-search list large enough for the autoindexing method to succeed. If the crystals have a similar orientation, using only very low resolution data may be the right method. In the case of twinned crystals, autoindexing sometimes finds a superlattice that results in integer indices simultaneously for both crystals. In such a case, *DENZO* solves the problem of finding the best three-dimensional lattice that incorporates all of the observed peaks. Unfortunately, for a twinned crystal, this is a mathematically correct solution to an incorrectly posed problem.

11.4.4. Coordinate systems

There are four natural coordinate systems used to describe a diffraction experiment, defined by the order in which the data are stored, the beam and gravity, or the beam and the goniostat axes (spindle or 2θ). These coordinate systems will be called, respectively, *data*, *beam–gravity*, *beam–spindle* and *beam–2θ*.

11.4.4.1. *Beam–gravity*

To visualize a diffraction pattern, beam–gravity is the coordinate system clearly preferred by human physiology. The universal preference to relate to the gravity direction is revealed by the observation that people generally perceive an image in a mirror as inverted left–right rather than top–down. Hence *XdisplayF* uses the beam–gravity coordinate system, except when diffraction data cannot be related to gravity.*

11.4.4.2. *Data*

The first (1983) *DENZO* implementation used the data coordinate system to describe the beam position on the detector and to define the integration box. This is still the case in order to keep backward compatibility.

11.4.4.3. *Beam–spindle*

Until 1998, *DENZO* supported only a single-axis goniostat and used a beam–spindle coordinate system to define crystal and detector orientation and polarization. Initially, the goniostat spindle axis was assumed to be horizontal, so the direction perpendicular to the beam and spindle was described by the keyword *vertical*, which in reality may not relate to the gravity direction for some goniostats. The keyword *rotx* relates to rotation around the spindle axis, *roty* around the *vertical axis* and *rotz* around the beam axis. The definition of the orientation matrix in the communication file between *DENZO* and *SCALEPACK* uses an unintuitive convention: the letter *y* in *roty* relates to the first element of the vector, *x* in *rotx* relates to the second and *z* in *rotz* to the third. However, the matrix always has a positive determinant, so this convention has no impact on the handedness of the coordinate system. This unfortunate choice of convention, preserved for backward compatibility reasons, appears only in the communication file and has no significance for anybody who does not inspect the matrix.

11.4.4.4. *Beam–2θ*

The recent addition of a general goniostat introduced a conceptual change in the *DENZO* coordinate system. The data-collection axis can be oriented in any direction, so in principle *rotx*, *roty* and *rotz* no longer need to be defined relative to the data-collection axis. However, to keep the useful correlation between refinable parameters (*crystal rotz* and *detector rotz* being close to 100% correlated), one real and two virtual goniostats are used simultaneously in *DENZO*. Refinable crystal parameters (*crystal rotx*, *roty*, *rotz*) are still defined, as in the past, by the data-collection axis and the beam. This means that the directions of rotations defined by *fit crystal rotx*, *roty* and *rotz* do not rotate around the data-collection axis as the program advances from one image to another. This coordinate system changes with the change in direction of the data-collection axis. Crystal orientation is defined by three constant, perpendicular axes, which, in the current version, no longer have to be aligned with the physical crystal goniostat. However, the so-called *2 theta* rotation has a fixed axis, and, if it exists, it defines the *DENZO* coordinate system together with the beam axis. Thus the current coordinate system in *DENZO* should be called beam–2θ. Fortunately for the user, the conversions between different coordinate systems are handled transparently. For example, the refined change in the crystal orientation is converted from the refined goniostat to the crystal-orientation goniostat. The

* There may occasionally be an exception to this when the experimental system is not known.

references