(in the manner described hereinbelow) which transform the Z cell edges ZA, ZB and ZC into the Y cell edges YA, YB and YC, respectively, within the respective specified tolerance values TOLI1, TOLI2 and TOLI3.

Next, the number of matrix triples determined in step **30** is tested in steps **40***a* and **40***b* to determine whether no matrix triples were found (step **40***a*) or a number of matrix triples were found exceeding a predetermined limit (e.g. 2000) (step **40***b*). If no matrix triples were found, further computations are terminated and a new cell Y is selected for comparison with cell Z in step **50***a* (when the identity of the lattice structure corresponding to cell Z is being sought). If too many matrix triples are found, further computations are terminated and an error signal is produced in step **50***b*.

If at least one set, but not an excessive number, of matrix triples are found in step **30**, then all combinations of those matrix triples found in step **30** are determined in step **60** (in the manner described hereinbelow) which also transform the Z cell angles ZAL, ZBE and ZGA into the Y cell angles YAL, YBE and YGA, respectively, within the respective specified tolerance values TOLI4, TOLI5 and TOLI6. Each combination of matrix triples found is saved as the elements U1, V1, W1, U2, V2, W2, U3, V3, W3 of a transformation matrix H.

The actual tolerances TOLA, TOLB, TOLC, TOLAL, TOLBE, TOLGA for each transformation matrix H determined in step **60** are calculated in step **70**, and the inverse H′ of each matrix H is calculated in step **80**.

Referring to FIG. **3**, a preferred method for determining the matrix triples in step **30** will now be described. First, in step **301**, a set of a predetermined number NHEL of possible integer and rational number values HEL(JJ), HEL(KK), HEL(LL) (JJ, KK, LL=1,2 . . . NHEL) for the elements of a transformation matrix H are defined (stored). A typical range of values HEL is $-6 \leqq BEL \leqq 6$, including both the integer values ± 1, ± 2, ± 3, ± 4, ± 5, and ± 6, and the non-integer rational number inverses thereof, i.e., $\pm \frac{1}{2}$, $\pm \frac{1}{3}$, $\pm \frac{1}{4}$, $\pm 1/5$ and $\pm 1/6$. The range of values HEL is normally selected based on the type of problem to be solved. With reduced versions of cells Y and Z, for example, the range of potential values for values HEL is reduced. In addition, variable indicies ICTMA, ICTMB and ICTMC, which are respectively used to identify the matrix triples AU, AV, AW; BU, BV, BW; and CU, CV, CW determined to transform the respective Z-cell edges into the corresponding Y-cell edges within the respective specified tolerances, as described hereinabove, are initialized to zero.

In steps **302–310**, variable indices JJ, KK and LL for signifying individual ones of the values HEL and controlling iteration of computation loops are initialized, incremented and compared with NHEL in the sequence shown to provide first, second and third nested computation loops using successive combinations of HEL(JJ), HEL(KK) and HEL(LL) as described in more detail hereinbelow.

Since JJ, KK, and LL initially are not greater than NHEL, as determined in steps **304**, **307** and **310**, respectively, a symmetrical dot product TZEE for transformed cell Z is calculated in step **312** using values HEL(JJ), HEL(KK) and HEL(LL) and dot products **Z11**, **Z22**, **Z33**, **Z23**, **Z13** and **Z12** for cell Z calculated in step **20** (FIG. **2**) as follows:

$$TZEE = HEL(JJ)*HEL(JJ)*Z11 + HEL(KK)*HEL(KK)*Z22 + HEL(LL)*HEL(LL)*Z33 + 2.0\,(HEL(KK)*HEL(LL)*Z23 + HEL(JJ)*HEL(LL)*Z13 + HEL(JJ)*HEL(KK)*Z12)$$

It will be appreciated that the values HEL(JJ), HEL(KK) and HEL(LL) form a row of a transformation matrix and that the calculated dot product may correspond to A.A, B.B or C.C depending on the order of the matrix row in the final transformation matrix H.

Next, in step **314**, dot product TZEE is tested to determine whether it is greater than zero. If not, no further computations are done using the current combination of values HEL, and the third computation loop comprising steps **309–346** is restarted using a new value of HEL(LL) by returning to step **309**.

If TZEE>0, then a transformed edge for cell Z, TZEDG, is derived (step **316**) as follows:

$$TZEDG = \sqrt{TZEE}$$

Then TZEDG is tested (step **318**) to determine whether it constitutes a transformation of Z-cell edge ZA to Y-cell edge YA within the specified tolerance TOLI1 by determining whether:

$$(TOLI1 - |TZEDG - YA|) < 0.$$

If the determination in step **318** is TRUE (i.e., the foregoing inequality is FALSE) then the current values of HEL(JJ), HEL(KK) and HEL(LL) from which TZEDG was derived is a possible row in a transformation matrix H; and the counter ICTMA is thus incremented (step **320**), and the values HEL(JJ), HEL(KK) and HEL(LL) are saved (step **322**) as matrix triple AU(ICTMA), AV(ICTMA) and AW(ICTMA), respectively. A value DA(ICTMA)=TZEDG−YA representing the actual tolerance (difference) between the transformed Z cell edge A and the inputted Y-cell YA is also calculated and saved (step **324**); together with a value TZA(ICTMA)=TZEDG as the transformed Z-cell edge a parameter (step **326**). The computation then proceeds to step **328**.

If a FALSE determination is made in step **318** (i.e., the inequality is TRUE), then TZEDG is similarly tested in step **328** to determine whether it constitutes a transformation of the Z-cell edge ZB to the Y-cell edge YB within the specified tolerance TOL12, i.e., whether (TOLI2−|TZEDG−YB|)<O. Similarly to steps **320–326**, if the determination in step **328** is TRUE, then the counter ICTMB is incremented (step **330**); the current values of HEL(JJ), HEL(KK) and HEL(LL) are saved (step **332**) as matrix triple BU(ICTMB), BV(ICTMB), BW(ICTMB); values DB(ICTMB)=-TZEDG−YB, and TZB(ICTMB)=TZEDG are calculated and saved (steps **334–336**); and the computation proceeds to step **338**.

If a FALSE determination is made in step **328**, then TZEDG is again similarly tested in step **338** with respect to Y-cell edge YC to determine whether (TOLI3-|TZEDG-YB|)<O. Similarly to steps **320–326** and **330–336**, if the determination in step **338** is TRUE, then counter ICTMC is incremented (step **340**); the current values of HEL(JJ), HEL(KK) and HEL(LL) are saved (step **342**) as matrix triple CU(ICTMC), CV(ICTMC),