

and if not, converting alpha value cos4 to an angle value TZAL;
 determining whether TZAL is within said maximum allowable tolerance TOL14, and if so, deriving a beta value cos5 for said transformed cell TZ;
 determining whether beta value cos5 is greater than or equal to +1 or less than or equal to -1, and if not, converting beta value cos5 to an angle value TZBE;
 determining whether TZBE is within said maximum allowable tolerance TOL14, and if so, saving the combination of matrix triples as the elements U1, V1, W1, U2, V2, W2, U3, V3 and W3 of a transformation matrix H.
 34. The apparatus of claim 31 wherein said gamma value cos6 is derived by:
 determining a value $TZEF1 = AU(J) * BU(K) * Z1 + AV(J) * BV(K) * Z22 + AW(J) * BW(K) * Z33 + (AV(J) * BW(K) + AW(J) * BV(K)) * Z23 + (AU(J) * BW(K) + AW(K) * BU(K)) * Z13 + (AU(J) * BV(K) + AV(J) * BU(-K)) * Z12$; and
 deriving gamma value $cos6 = TZEF1 / (-TZA(J) * TZB(K))$.
 35. The apparatus of claim 31 wherein said alpha value cos4 is derived by:
 determining a value $TZEF2 = BU(K) * CU(L) * Z11 + BV(K) * CV(L) * Z22 + BW(K) * CW(L) * Z33 + (BV(K) * CW(L) + BW(K) * -CV(L)) * Z23 + (BU(K) * CW(L) + BW(K) * CU(L)) * Z13 + (BU(K) * CV(L) + BV(K) * CU(L)) * Z12$; and
 deriving alpha value $cos4 = -TZEF2 / (TZB(K) * TZC(L))$.
 36. The apparatus of claim 31 wherein said beta value cos5 is derived by:
 determining a value $TZEF3 = AU(J) * CU(L) * Z11 + AV(J) * CV(L) * Z22 + AW(J) * CW(L) * Z33 + (AV(J) * CW(L) + AW(J) * -CV(L)) * Z23 + (AU(J) * CW(L) + AW(J) * CU(L)) * Z13 + (AU(J) * CV(L) + AV(J) * CU(L)) * Z12$; and
 deriving beta value $cos5 = TZEF3 / (-TZA(J) * TZC(L))$.
 37. Automatic apparatus for identifying an unknown crystalline material comprising:
 an electronic signal analyzer, responsive to electrical signals generated by detecting radiation received

from a sample of the unknown material which has been irradiated by radiation, for producing electrical data signal outputs indicative of a primitive lattice cell Z of the unknown material, said cell Z having three cell edges ZA, ZB and ZC, respectively, and three cell angles ZAL, ZBE, and ZGA, respectively;
 a first computer accessible memory in which is stored a database for materials with known lattice structures and chemical compositions, said database comprising lattice cell data and element type data identifying the lattice structures and chemical compositions, respectively, of the database materials;
 first computer search means responsive to said electronic signal analyzer data signal outputs for automatically searching said database using a converse transformation method to generate matrices H identifying all materials, if any, having lattice cell structures related to cell Z;
 computer means for analyzing any matrices H generated by said first search means to identify which of the database materials identified by the generated matrices H match cell Z by having a lattice cell structure identical to or in a subcell/supercell derivative relationship to cell Z, any database material so identified as matching cell Z constituting a possible identification of the unknown crystalline material;
 means for determining the element types identifying the chemical composition of the unknown material and producing electrical signal outputs indicative of the unknown material element types;
 second computer search means responsive to the electrical signal outputs produced by said element type determining means for automatically searching said database for all compounds which match the unknown material by having the same or related element types as the unknown material;
 a computer accessible second memory for saving as a first data set the compounds matching cell Z identified by said matrix H analyzing means, and as a second data set the matching compounds with the same element types as the unknown material identified by said second search means; and
 said computer means includes means for combining said first and second data sets stored in said electronic memory to derive all known compounds having the same lattice cell structure and element types as the unknown material.
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