Fig. 4

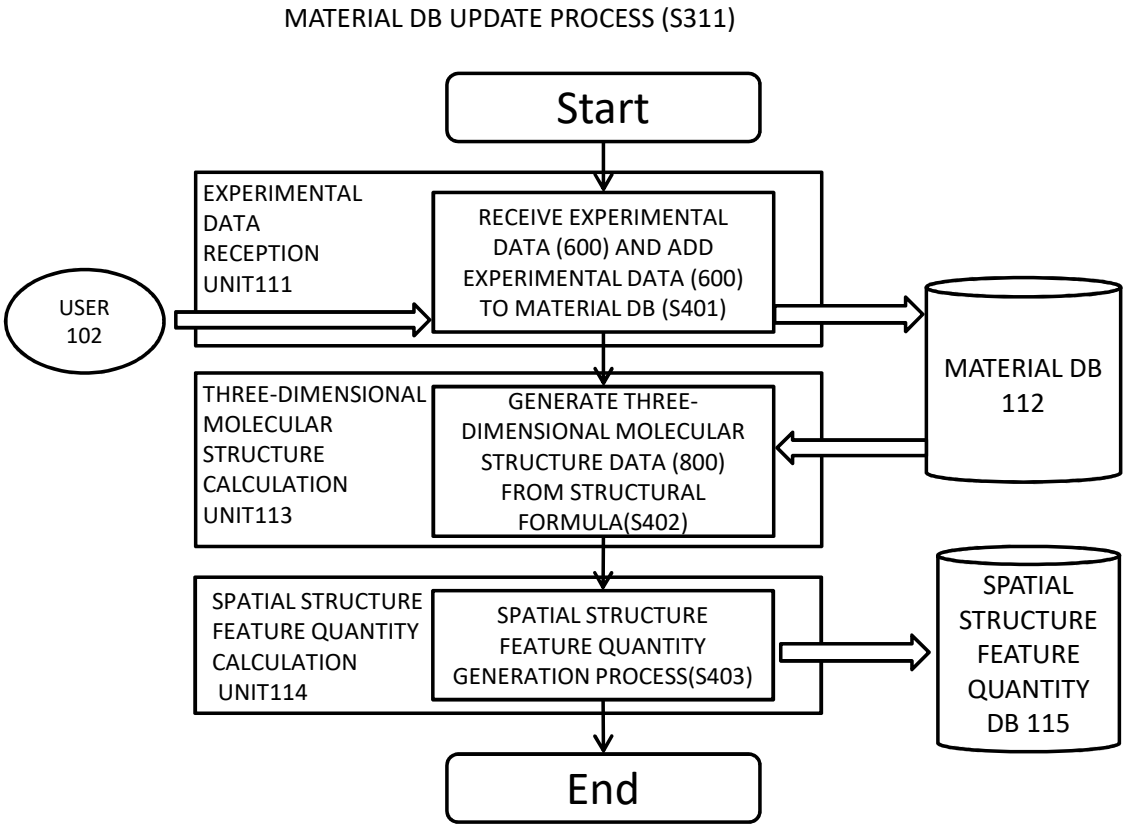

MATERIAL DB UPDATE PROCESS (S311)
Start
EXPERIMENTAL DATA RECEPTION UNIT111
RECEIVE EXPERIMENTAL DATA (600) AND ADD EXPERIMENTAL DATA (600) TO MATERIAL DB (S401)
USER 102
MATERIAL DB 112
THREE-DIMENSIONAL MOLECULAR STRUCTURE CALCULATION UNIT113
GENERATE THREE-DIMENSIONAL MOLECULAR STRUCTURE DATA (800) FROM STRUCTURAL FORMULA(S402)
SPATIAL STRUCTURE FEATURE QUANTITY CALCULATION UNIT114
SPATIAL STRUCTURE FEATURE QUANTITY GENERATION PROCESS(S403)
SPATIAL STRUCTURE FEATURE QUANTITY DB 115
End

Fig. 12

TABLE OF SPATIAL STRUCTURE FEATURE QUANTITY (1200)

ITEM NAME	***CONTENTS***
EXPERIMENT ID(701)	IDENTIFICATION NUMBER UNIQUELY IDENTIFYING EXPERIMENT
INFORMATION (1201) OF REFERENCE ATOM 1	ATOMIC NUMBER OF REFERENCE ATOM 1
INFORMATION (1202) OF REFERENCE ATOM 2	ATOMIC NUMBER OF REFERENCE ATOM 2
INFORMATION (1203) OF REFERENCE ATOM 3	ATOMIC NUMBER OF REFERENCE ATOM 3
DISTANCE (1204) BETWEEN REFERENCE ATOMS 1 AND 2	EUCLIDEAN DISTANCE BETWEEN REFERENCE ATOMS 1 AND 2
DISTANCE (1205) BETWEEN REFERENCE ATOMS 2 AND 3	EUCLIDEAN DISTANCE BETWEEN REFERENCE ATOMS 2 AND 3
DISTANCE (1206) BETWEEN REFERENCE ATOMS 1 AND 3	EUCLIDEAN DISTANCE BETWEEN REFERENCE ATOMS 1 AND 3
DISTANCE d1 (1207) OF FIRST ATOM FROM REFERENCE ATOM 1	EUCLIDEAN DISTANCE BETWEEN FIRST ATOM AND REFERENCE ATOM 1. 0 WHEN NUMBER OF ATOMS CONSTITUTING MOLECULE IS SMALLER THAN N
DISTANCE (1208) OF FIRST ATOM FROM REFERENCE ATOM 2	EUCLIDEAN DISTANCE BETWEEN FIRST ATOM AND REFERENCE ATOM 2. 0 WHEN NUMBER OF ATOMS CONSTITUTING MOLECULE IS SMALLER THAN N
DISTANCE (1209) OF FIRST ATOM FROM REFERENCE ATOM 3	EUCLIDEAN DISTANCE BETWEEN FIRST ATOM AND REFERENCE ATOM 3. 0 WHEN NUMBER OF ATOMS CONSTITUTING MOLECULE IS SMALLER THAN N
...	...
DISTANCE OF N-TH ATOM FROM REFERENCE ATOM 1	EUCLIDEAN DISTANCE BETWEEN N-TH ATOM AND REFERENCE ATOM 1. 0 WHEN NUMBER OF ATOMS CONSTITUTING MOLECULE IS SMALLER THAN N
DISTANCE OF N-TH ATOM FROM REFERENCE ATOM 2	EUCLIDEAN DISTANCE BETWEEN N-TH ATOM AND REFERENCE ATOM 2. 0 WHEN NUMBER OF ATOMS CONSTITUTING MOLECULE IS SMALLER THAN N
DISTANCE OF N-TH ATOM FROM REFERENCE ATOM 3	EUCLIDEAN DISTANCE BETWEEN N-TH ATOM AND REFERENCE ATOM 3. 0 WHEN NUMBER OF ATOMS CONSTITUTING MOLECULE IS SMALLER THAN N

Fig. 13

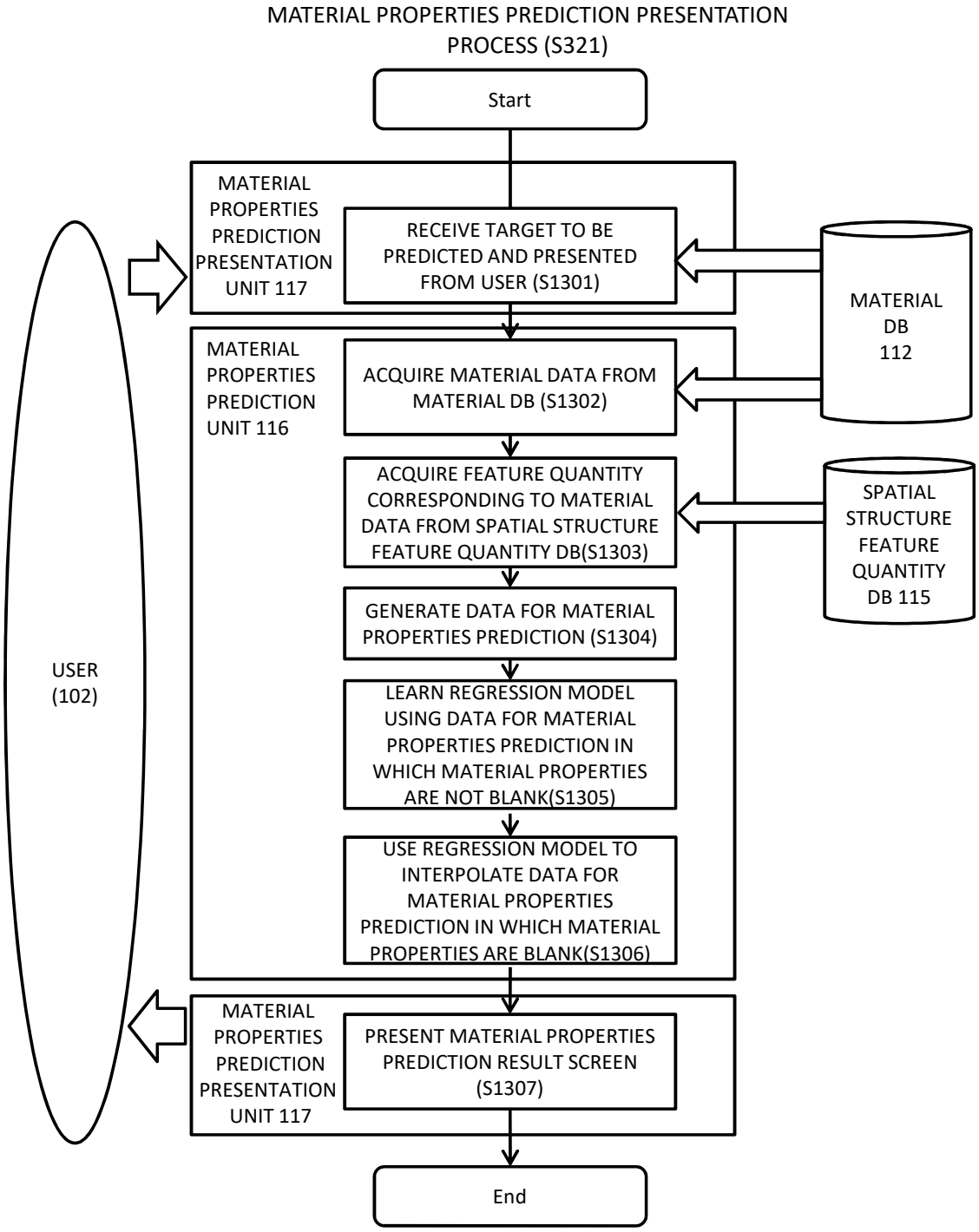
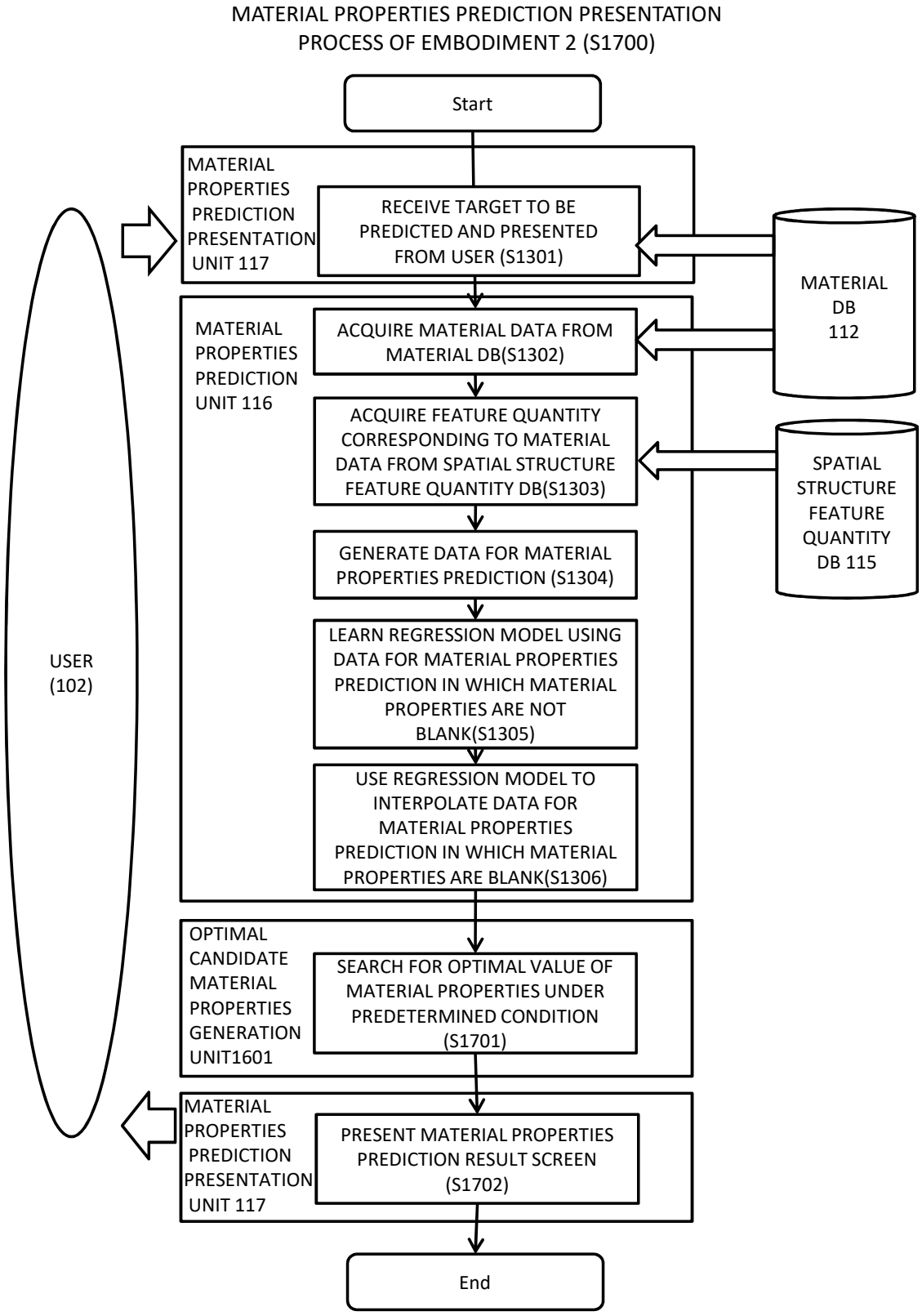

MATERIAL PROPERTIES PREDICTION PRESENTATION PROCESS (S321)
Start
MATERIAL PROPERTIES PREDICTION PRESENTATION UNIT 117
RECEIVE TARGET TO BE PREDICTED AND PRESENTED FROM USER (S1301)
MATERIAL DB 112
MATERIAL PROPERTIES PREDICTION UNIT 116
ACQUIRE MATERIAL DATA FROM MATERIAL DB (S1302)
ACQUIRE FEATURE QUANTITY CORRESPONDING TO MATERIAL DATA FROM SPATIAL STRUCTURE FEATURE QUANTITY DB(S1303)
SPATIAL STRUCTURE FEATURE QUANTITY DB 115
GENERATE DATA FOR MATERIAL PROPERTIES PREDICTION (S1304)
LEARN REGRESSION MODEL USING DATA FOR MATERIAL PROPERTIES PREDICTION IN WHICH MATERIAL PROPERTIES ARE NOT BLANK(S1305)
USE REGRESSION MODEL TO INTERPOLATE DATA FOR MATERIAL PROPERTIES PREDICTION IN WHICH MATERIAL PROPERTIES ARE BLANK(S1306)
USER (102)
MATERIAL PROPERTIES PREDICTION PRESENTATION UNIT 117
PRESENT MATERIAL PROPERTIES PREDICTION RESULT SCREEN (S1307)
End

Fig. 15

ONE RECORD OF DATA FOR MATERIAL PROPERTIES PREDICTION(1500)

ITEM NAME	***CONTENTS***
EXPERIMENT ID(701)	IDENTIFICATION NUMBER UNIQUELY IDENTIFYING EXPERIMENT
MATERIAL PROPERTIES(702)	VALUE INDICATING MATERIAL PROPERTIES. BLANK FOR NON-MEASUREMENT
EXPERIMENTAL CONDITION(704)	CONDITION VALUE OTHER THAN STRUCTURAL FORMULA OF MATERIAL
INFORMATION (1201) OF REFERENCE ATOM 1	ATOMIC NUMBER OF REFERENCE ATOM 1
INFORMATION (1202) OF REFERENCE ATOM 2	ATOMIC NUMBER OF REFERENCE ATOM 2
INFORMATION (1203) OF REFERENCE ATOM 3	ATOMIC NUMBER OF REFERENCE ATOM 3
DISTANCE (1204) BETWEEN REFERENCE ATOMS 1 AND 2	UCLIDEAN DISTANCE BETWEEN REFERENCE ATOMS 1 AND 2
DISTANCE (1205) BETWEEN REFERENCE ATOMS 2 AND 3	UCLIDEAN DISTANCE BETWEEN REFERENCE ATOMS 2 AND 3
DISTANCE (1206) BETWEEN REFERENCE ATOMS 1 AND 3	UCLIDEAN DISTANCE BETWEEN REFERENCE ATOMS 1 AND 3
DISTANCE d1 (1207) OF FIRST ATOM FROM REFERENCE ATOM 1	EUCLIDEAN DISTANCE BETWEEN FIRST ATOM AND REFERENCE ATOM 1. 0 WHEN NUMBER OF ATOMS CONSTITUTING MOLECULE IS SMALLER THAN N
DISTANCE (1208) OF FIRST ATOM FROM REFERENCE ATOM 2	EUCLIDEAN DISTANCE BETWEEN FIRST ATOM AND REFERENCE ATOM 2. 0 WHEN NUMBER OF ATOMS CONSTITUTING MOLECULE IS SMALLER THAN N
DISTANCE (1209) OF FIRST ATOM FROM REFERENCE ATOM 3	EUCLIDEAN DISTANCE BETWEEN FIRST ATOM AND REFERENCE ATOM 3. 0 WHEN NUMBER OF ATOMS CONSTITUTING MOLECULE IS SMALLER THAN N
...	...
DISTANCE OF N-TH ATOM FROM REFERENCE ATOM 1	EUCLIDEAN DISTANCE BETWEEN N-TH ATOM AND REFERENCE ATOM 1. 0 WHEN NUMBER OF ATOMS CONSTITUTING MOLECULE IS SMALLER THAN N
DISTANCE OF N-TH ATOM FROM REFERENCE ATOM 2	EUCLIDEAN DISTANCE BETWEEN N-TH ATOM AND REFERENCE ATOM 2. 0 WHEN NUMBER OF ATOMS CONSTITUTING MOLECULE IS SMALLER THAN N
DISTANCE OF N-TH ATOM FROM REFERENCE ATOM 3	EUCLIDEAN DISTANCE BETWEEN N-TH ATOM AND REFERENCE ATOM 3. 0 WHEN NUMBER OF ATOMS CONSTITUTING MOLECULE IS SMALLER THAN N

Fig. 17


MATERIAL PROPERTIES PREDICTION PRESENTATION PROCESS OF EMBODIMENT 2 (S1700)
Start
MATERIAL PROPERTIES PREDICTION PRESENTATION UNIT 117
RECEIVE TARGET TO BE PREDICTED AND PRESENTED FROM USER (S1301)
MATERIAL DB 112
MATERIAL PROPERTIES PREDICTION UNIT 116
ACQUIRE MATERIAL DATA FROM MATERIAL DB(S1302)
ACQUIRE FEATURE QUANTITY CORRESPONDING TO MATERIAL DATA FROM SPATIAL STRUCTURE FEATURE QUANTITY DB(S1303)
SPATIAL STRUCTURE FEATURE QUANTITY DB 115
GENERATE DATA FOR MATERIAL PROPERTIES PREDICTION (S1304)
LEARN REGRESSION MODEL USING DATA FOR MATERIAL PROPERTIES PREDICTION IN WHICH MATERIAL PROPERTIES ARE NOT BLANK(S1305)
USE REGRESSION MODEL TO INTERPOLATE DATA FOR MATERIAL PROPERTIES PREDICTION IN WHICH MATERIAL PROPERTIES ARE BLANK(S1306)
USER (102)
OPTIMAL CANDIDATE MATERIAL PROPERTIES GENERATION UNIT1601
SEARCH FOR OPTIMAL VALUE OF MATERIAL PROPERTIES UNDER PREDETERMINED CONDITION (S1701)
MATERIAL PROPERTIES PREDICTION PRESENTATION UNIT 117
PRESENT MATERIAL PROPERTIES PREDICTION RESULT SCREEN (S1702)
End