

Fig. 1

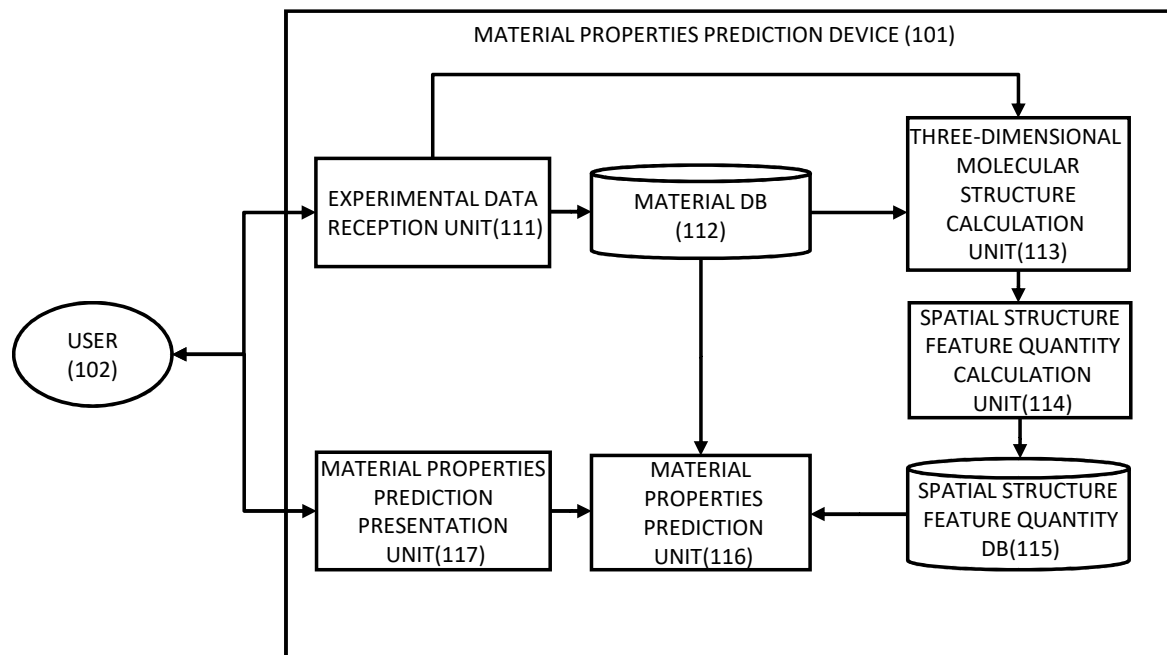


Fig. 2

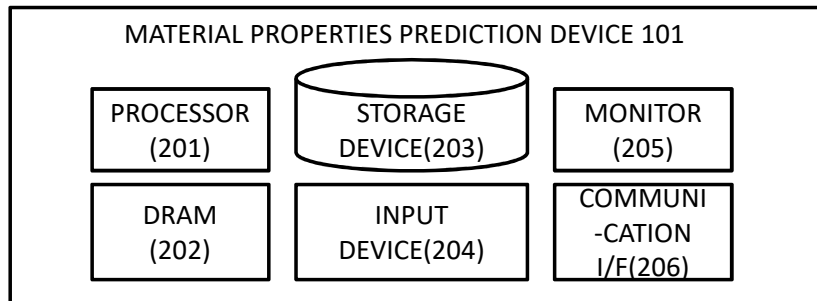


Fig. 3

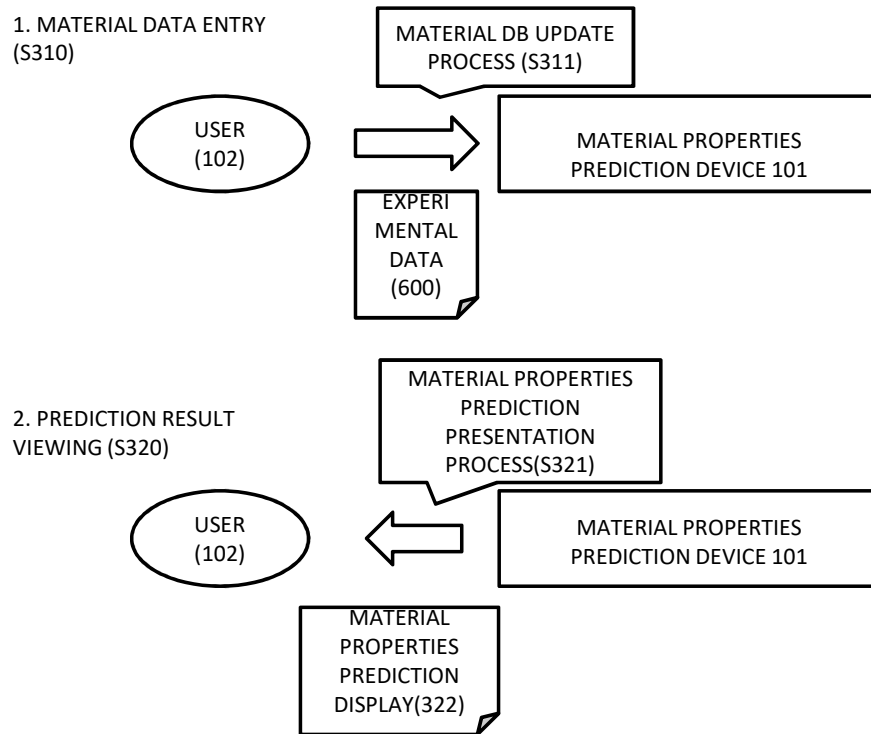


Fig. 4

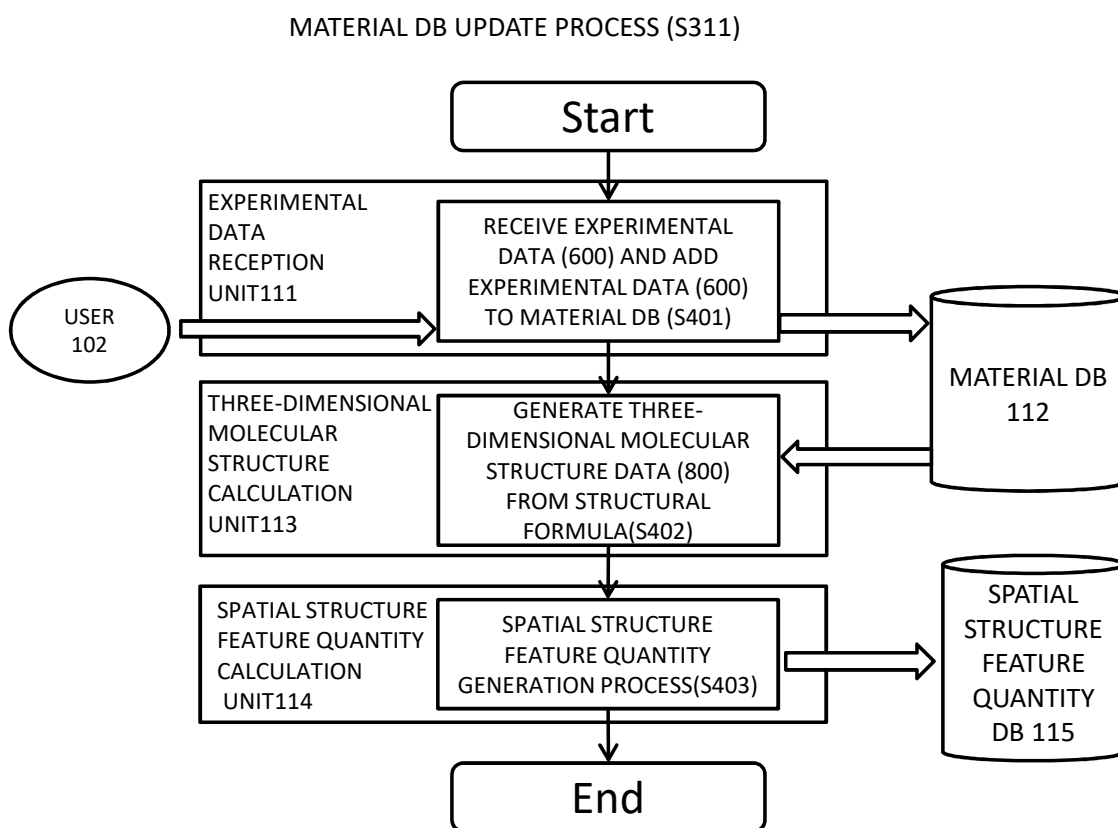


Fig. 5

DISPLAY SCREEN FOR RECEIVING EXPERIMENTAL DATA

501

502

503

DATA ENTRY

C:\work\hoge hoge\data.csv

REFERENCE

UPLOAD

ID	Temp	SOL	SMILES
10	98.1	11.2	CCCN
11	89.1	22.1	COOC=C
12	120.2	32.0	CNCNCC(OC)
13	84.1		OC(CCCCC)CCN
15	75.0	17.5	(CCCCC)O(CCCC)NC
18	100.2	26.7	CC

TABLE NAME : hogedata

STORE

CANCEL

Fig. 6

EXPERIMENTAL DATA (600)

<i>ITEM NAME</i>	<i>CONTENTS</i>
MATERIAL PROPERTIES (601)	VALUE INDICATING MATERIAL PROPERTIES. BLANK FOR NON-MEASUREMENT
MATERIAL STRUCTURAL FORMULA(602)	CHARACTER STRING INDICATING STRUCTURAL FORMULA OF MATERIAL
EXPERIMENTAL CONDITION (603)	CONDITION VALUE OTHER THAN STRUCTURAL FORMULA OF MATERIAL

Fig. 7

EXPERIMENTAL DATA TABLE OF MATERIAL DB (112)

<i>ITEM NAME</i>	<i>CONTENTS</i>
EXPERIMENT ID (701)	IDENTIFICATION NUMBER UNIQUELY IDENTIFYING EXPERIMENT
MATERIAL PROPERTIES (702)	VALUE INDICATING MATERIAL PROPERTIES. BLANK FOR NON-MEASUREMENT
MATERIAL STRUCTURAL FORMULA (703)	CHARACTER STRING INDICATING STRUCTURAL FORMULA OF MATERIAL
EXPERIMENTAL CONDITION (704)	CONDITION VALUE OTHER THAN STRUCTURAL FORMULA OF MATERIAL

Fig. 8

INFORMATION CORRESPONDING TO SINGLE MOLECULE
AND INCLUDED IN THREE-DIMENSIONAL MOLECULAR
STRUCTURE DATA (800)

<i>ITEM NAME</i>	<i>CONTENTS</i>
EXPERIMENT ID(701)	IDENTIFICATION NUMBER UNIQUELY IDENTIFYING EXPERIMENT
ATOMIC NUMBER OF FIRST ATOM	ATOMIC NUMBER OF FIRST ATOM
x COORDINATE OF FIRST ATOM	x RELATIVE COORDINATE OF FIRST ATOM
y COORDINATE OF FIRST ATOM	y RELATIVE COORDINATE OF FIRST ATOM
z COORDINATE OF FIRST ATOM	z RELATIVE COORDINATE OF FIRST ATOM
...	...
ATOMIC NUMBER OF N-TH ATOM	ATOMIC NUMBER OF N-TH ATOM
x COORDINATE OF N-TH ATOM	x RELATIVE COORDINATE OF N-TH ATOM
y COORDINATE OF N-TH ATOM	y RELATIVE COORDINATE OF N-TH ATOM
z COORDINATE OF N-TH ATOM	z RELATIVE COORDINATE OF N-TH ATOM

Fig. 9

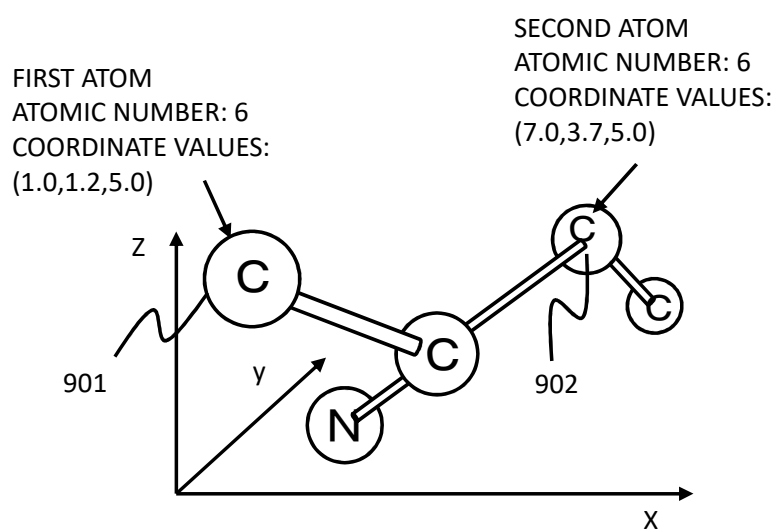


Fig. 10

SPATIAL STRUCTURE FEATURE QUANTITY CALCULATION PROCESS
(S403)

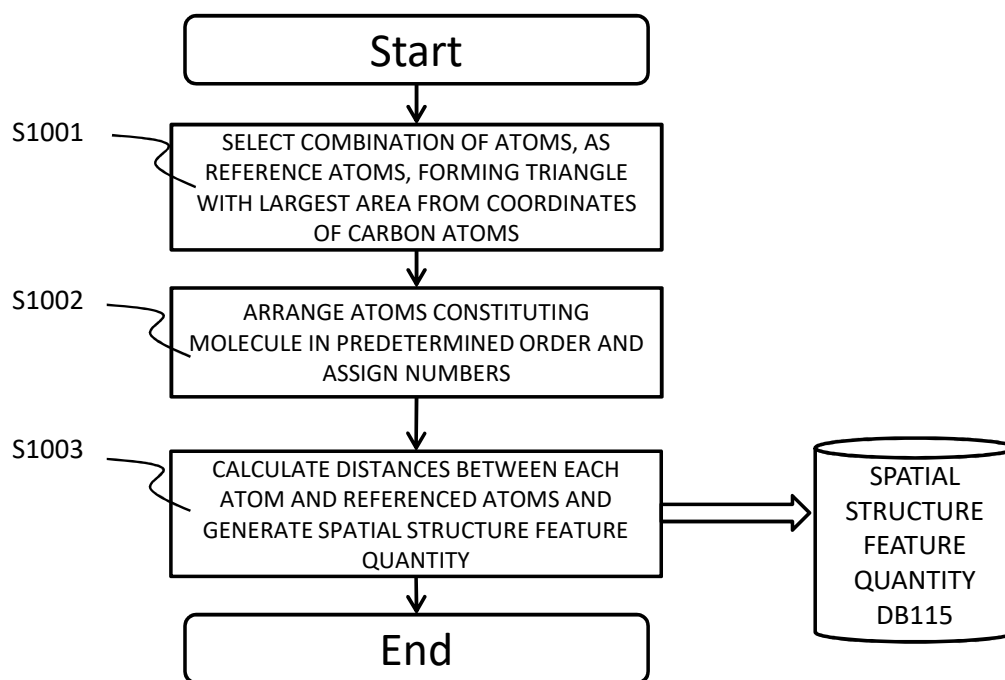


Fig. 11

MODEL FOR CALCULATING
SPATIAL STRUCTURE FEATURE
QUANTITY

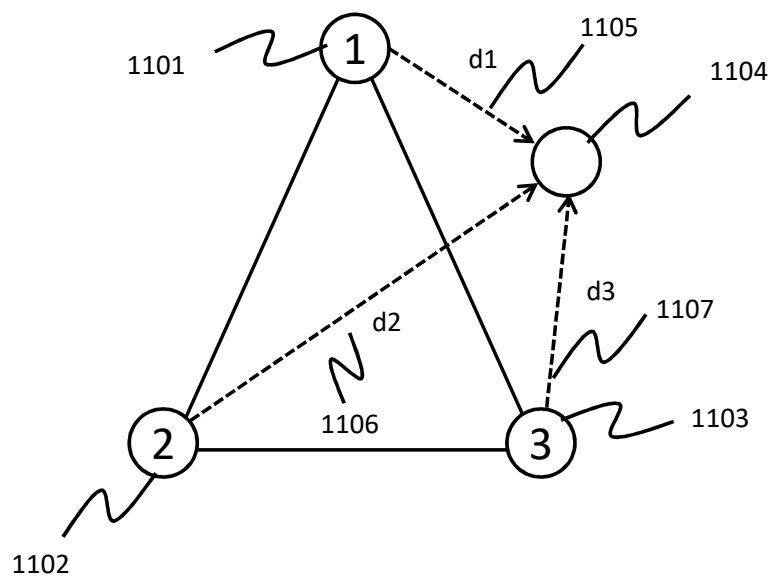


Fig. 12

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)

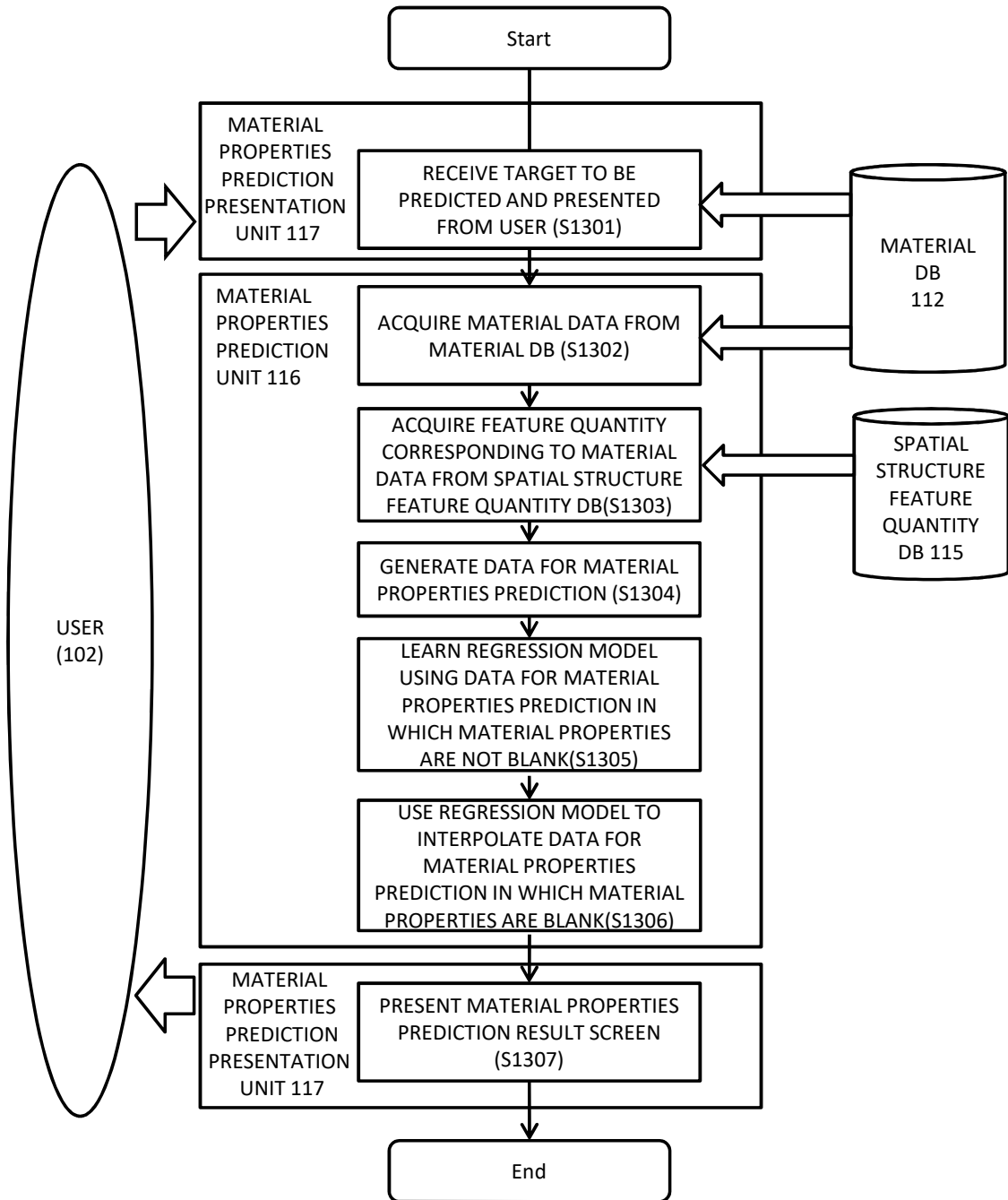


Fig. 14

1401

DATA ENTRY

MATERIAL DATA TABLE

tbl1

1402

UPDATE
PREDICTED VALUE

1403

ID	SMILES	T	MATERIAL PROPERTIES
1	C3O	10.2	10.2
2	C2OO	7.8	<u>7.8</u>
3	C2NO	10.2	10.2
4	COCOC	5.5	<u>5.5</u>
5	NCCI	10.1	10.1
6	CCCOC	17.2	17.2
7	CICCI	8.7	8.7

Fig. 15

ONE RECORD OF DATA FOR MATERIAL PROPERTIES PREDICTION(1500)

<i>ITEM NAME</i>	<i>CONTENTS</i>
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. 16

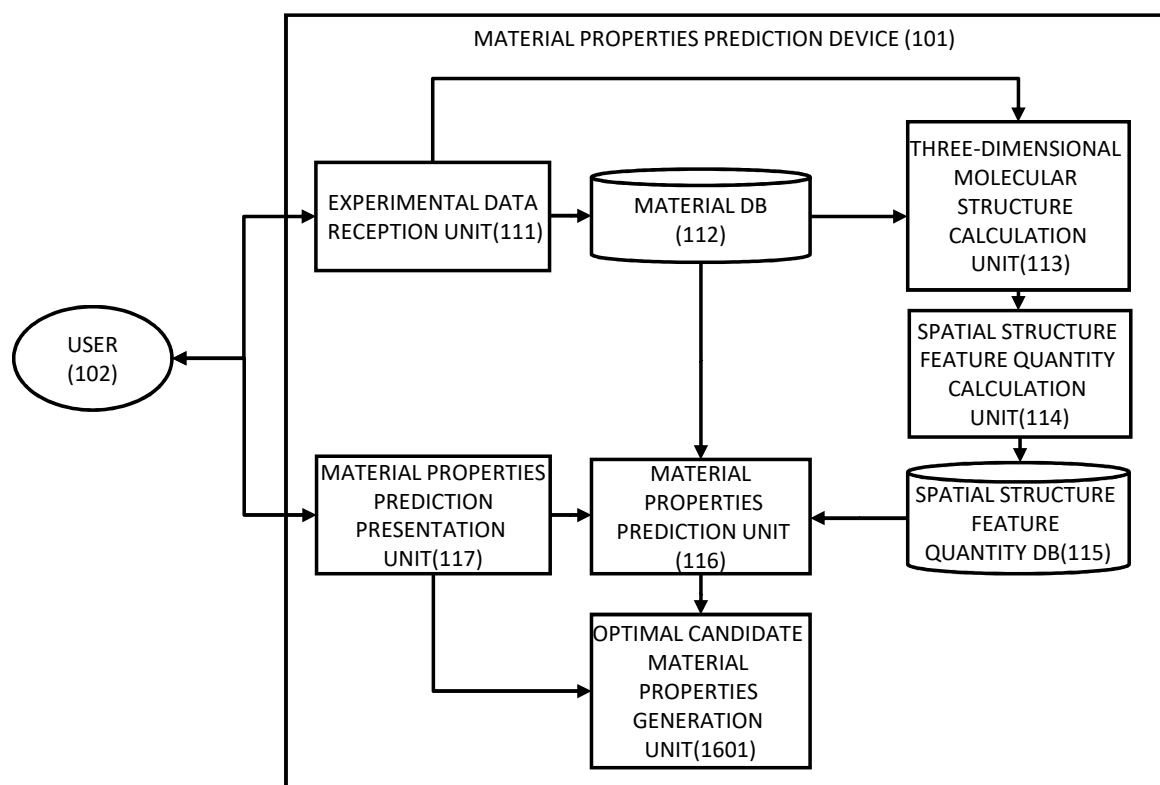


Fig. 17

MATERIAL PROPERTIES PREDICTION PRESENTATION
PROCESS OF EMBODIMENT 2 (S1700)

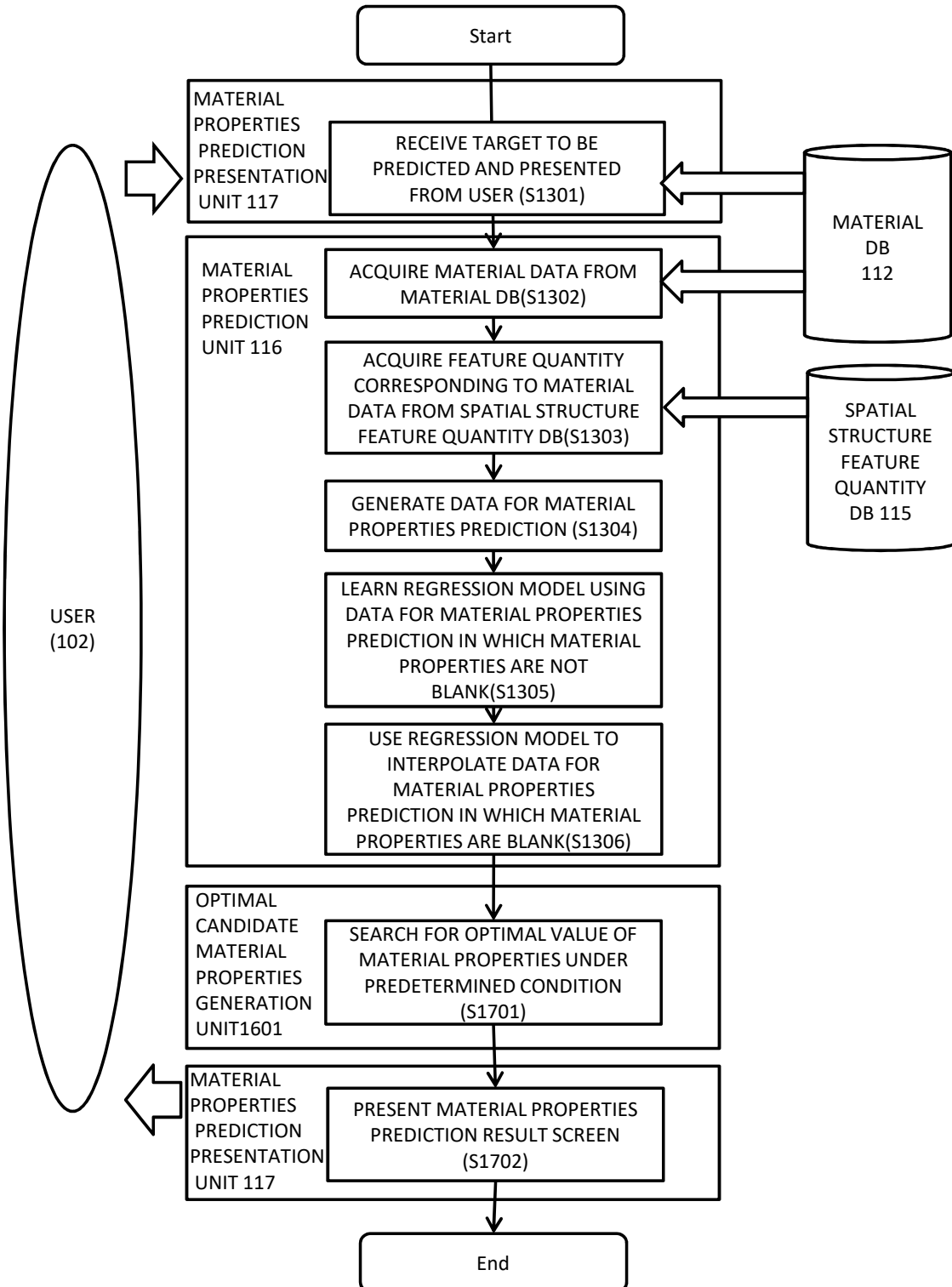


Fig. 18

