

Fig. 1

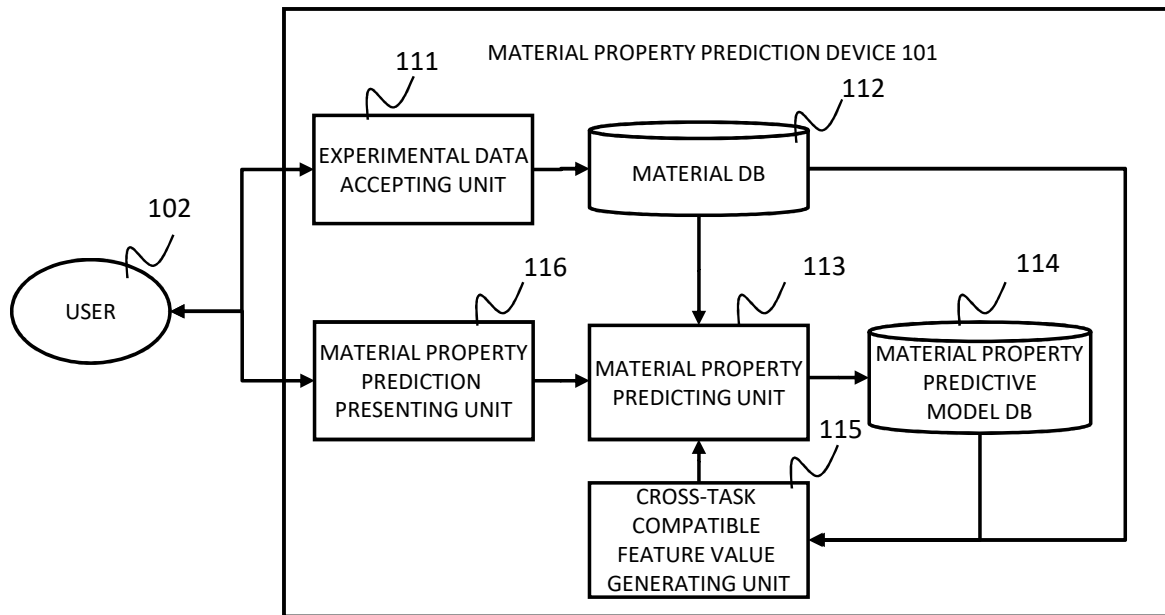


Fig. 2

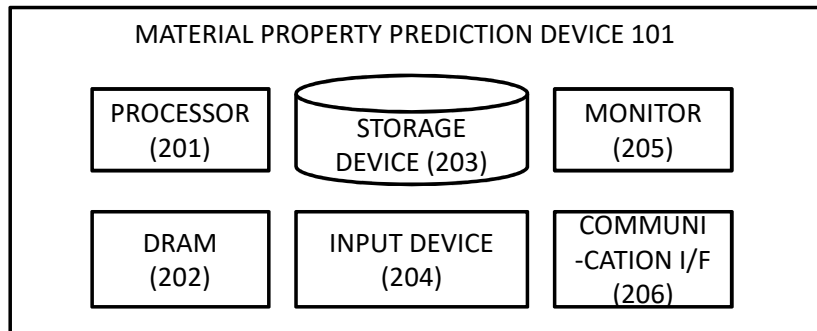


Fig. 3

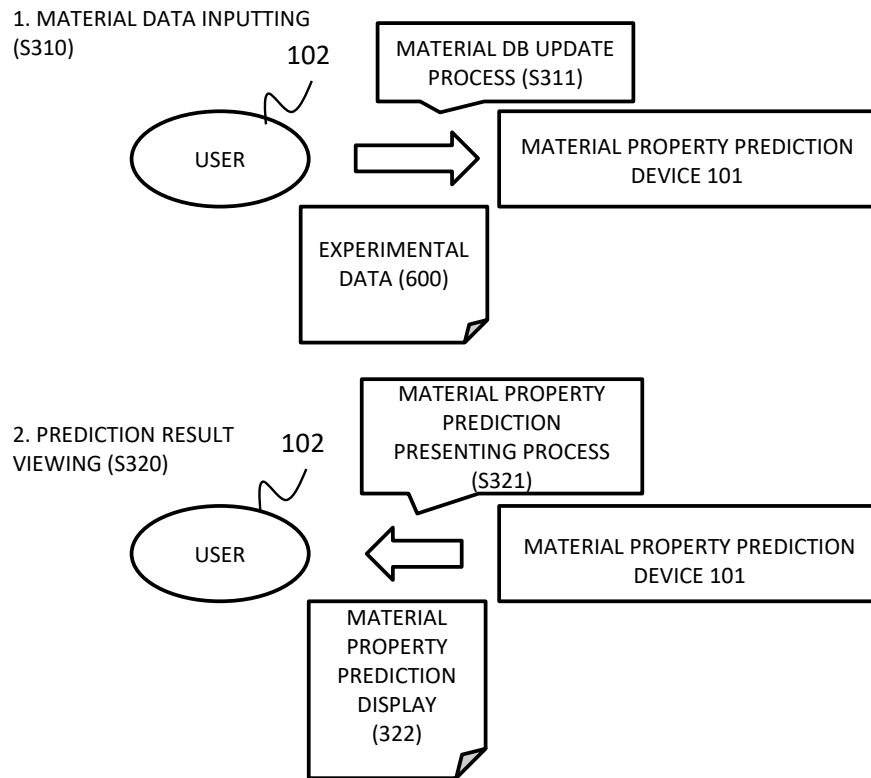


Fig. 4

MATERIAL DB UPDATE PROCESS (S311)

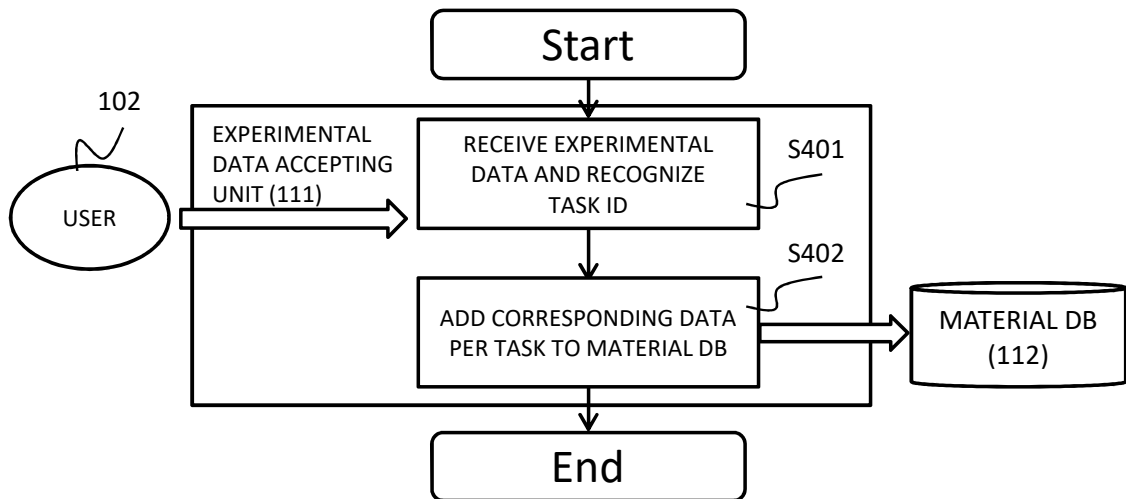


Fig. 5

SCREEN DISPLAYED FOR ACCEPTING
EXPERIMENTAL DATA

501

502

DATA INPUT

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

TASK NAME: hoge EXPERIMENT

SAVE

CANCEL

503

Fig. 6

EXPERIMENTAL DATA (600)

<i>ITEM NAME</i>	<i>DESCRIPTION</i>
MATERIAL PROPERTY (601)	VALUE INDICATING MATERIAL PROPERTY. BLANK FOR UNMEASURED PROPERTY
MATERIAL STRUCTURAL FORMULA (602)	STRING REPRESENTING MATERIAL STRUCTURAL FORMULA
EXPERIMENTAL CONDITION (603)	CONDITION NUMERICAL VALUE OTHER THAN MATERIAL STRUCTURAL FORMULA

Fig. 7

EXPERIMENTAL DATA TABLE IN MATERIAL DB (111)

<i>ITEM NAME</i>	<i>DESCRIPTION</i>
TASK ID (700)	IDENTIFICATION NUMBER THAT UNIQUELY IDENTIFIES TASK
EXPERIMENT ID (701)	IDENTIFICATION NUMBER THAT UNIQUELY IDENTIFIES EXPERIMENT
MATERIAL PROPERTY (702)	VALUE INDICATING MATERIAL PROPERTY. BLANK FOR UNMEASURED PROPERTY
MATERIAL STRUCTURAL FORMULA (703)	STRING REPRESENTING MATERIAL STRUCTURAL FORMULA
EXPERIMENTAL CONDITION (704)	CONDITION NUMERICAL VALUE OTHER THAN MATERIAL STRUCTURAL FORMULA

Fig. 8

PAST TASK A

ITEM NO.	STRUCTURAL FORMULA	EXPERIMENTAL CONDITION (TEMPERATURE)	<u>MATERIAL PROPERTY A</u>
1	CH ₃ COOH	18.1	<u>10</u>
2	CH ₃ CH ₂ OOH	20.5	<u>22</u>
3	OH-CH=CH-OH	19.7	<u>18</u>

PAST TASK B



ITEM NO.	STRUCTURAL FORMULA	EXPERIMENTAL CONDITION (HUMIDITY)	<u>MATERIAL PROPERTY B</u>
1	CH ₃ CNOH	98.0	<u>100</u>
2	NH=CHOOH	70.3	<u>202</u>
3	CH ₂ =CHOCH ₃	55.9	<u>181</u>
4	CH ₃ CH ₂ CH ₂ CH ₃	98.2	<u>PREDICTION TARGET</u>

Fig. 9

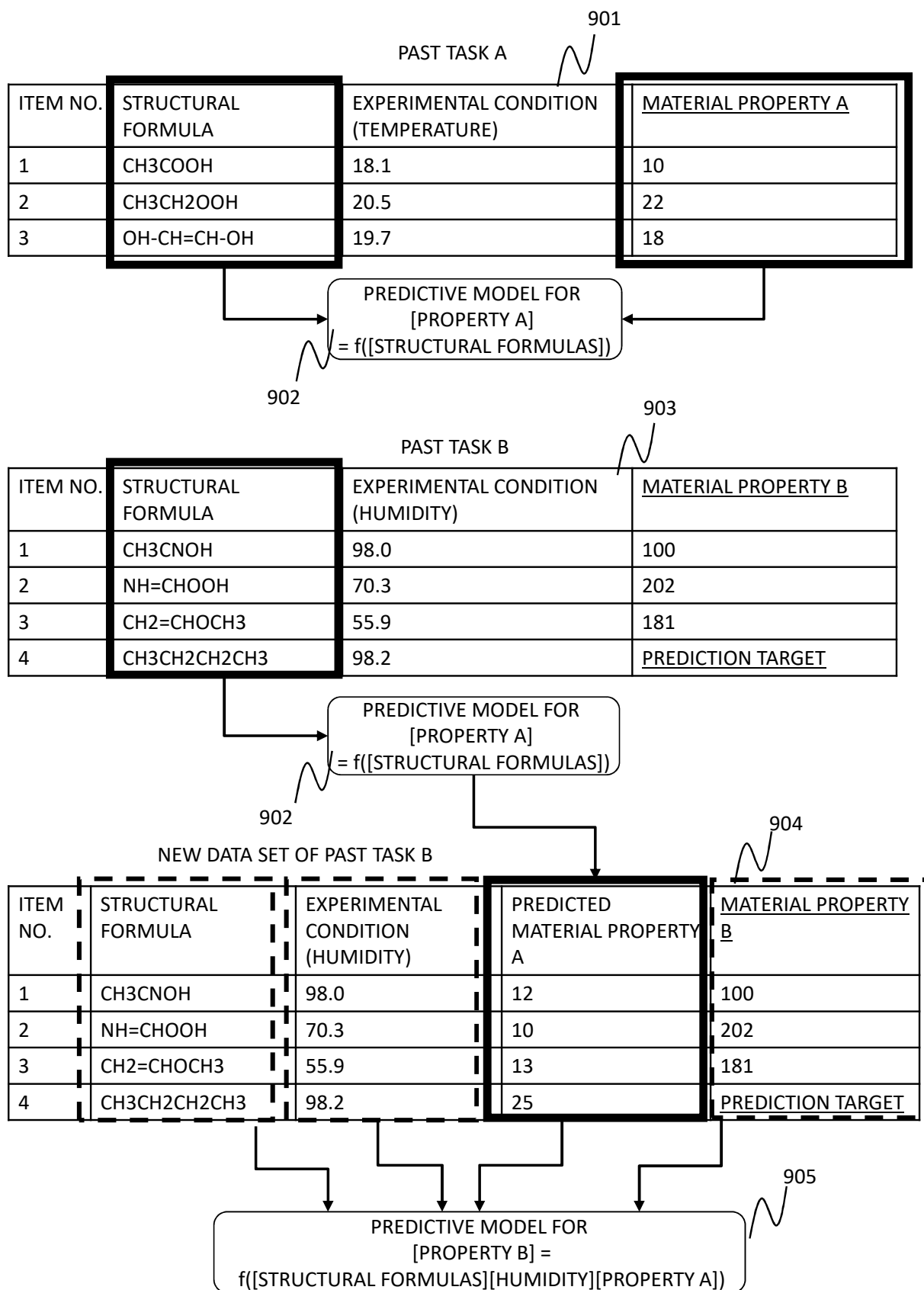


Fig. 10

MATERIAL PROPERTY PREDICTION PROCESS (S321)

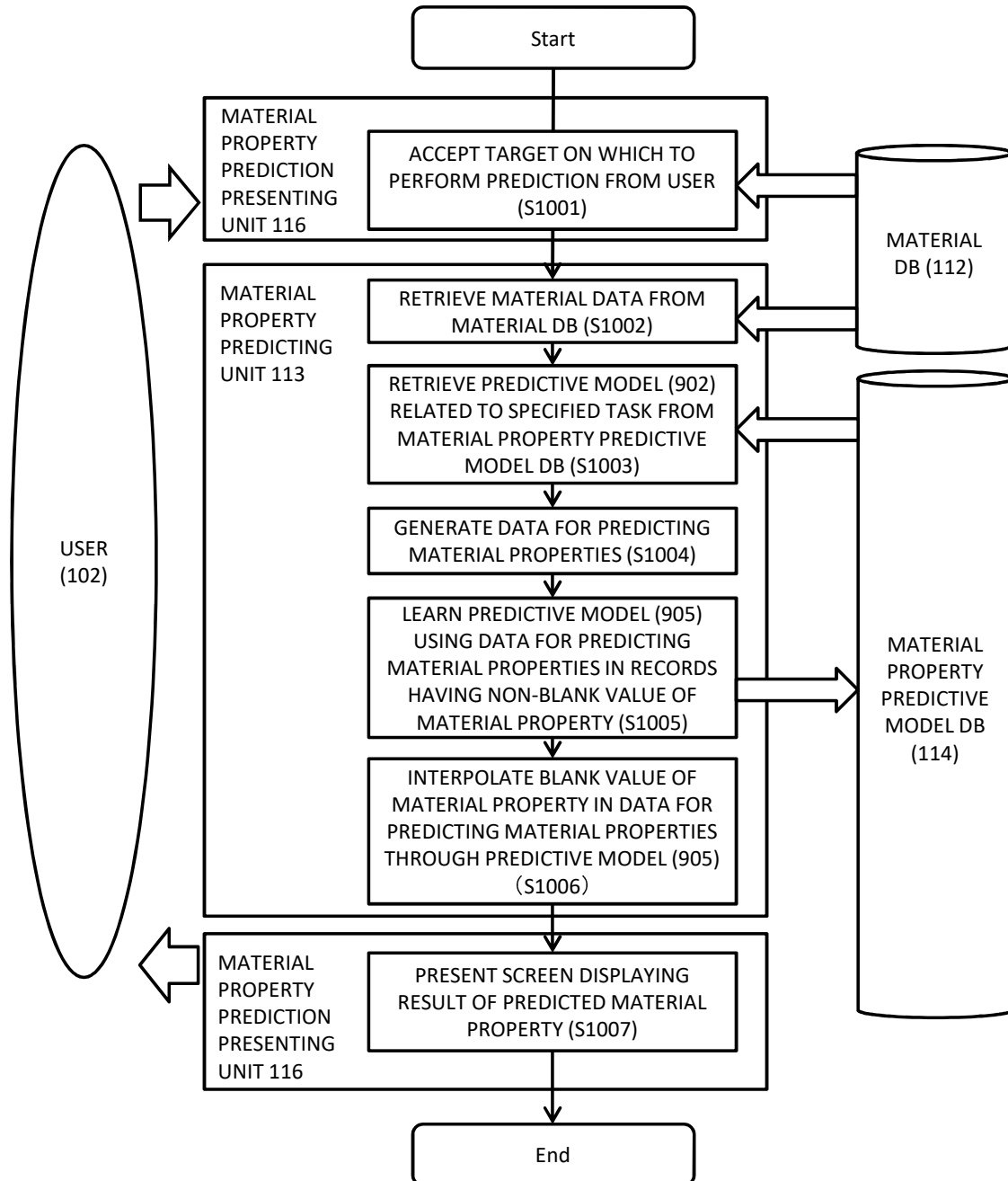


Fig. 11

DATA INPUT

MATERIAL DATA TABLE

tbl1

VIRTUAL MOLECULE WITH LARGEST MATERIAL PROPERTY

ADD

INFORMATION ON ANY OTHER TASK TO BE USED FOR PREDICTION

DELETE SELECTED TASK

TASK ~ ~ ~ ~

TASK *** ON ~ ~ ~ ~

x O x O O x x x x x O

PREDICTED VALUE UPDATE

ID	SMILES	T	MATERIAL PROPERTY
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	CCOC	17.2	17.2
7	CICCI	8.7	8.7

Fig. 12

ONE RECORD OF DATA FOR PREDICTING MATERIAL PROPERTIES(1500)

<i>ITEM NAME</i>	<i>DESCRIPTION</i>
TASK ID (700)	IDENTIFICATION NUMBER THAT UNIQUELY IDENTIFIES TASK
EXPERIMENT ID (701)	IDENTIFICATION NUMBER THAT UNIQUELY IDENTIFIES EXPERIMENT
MATERIAL PROPERTY (702)	VALUE INDICATING MATERIAL PROPERTY. BLANK FOR UNMEASURED PROPERTY
FEATURE VALUES DERIVED FROM STRUCTURAL FORMULAS (1201)	FEATURE VALUES COMPUTED FROM STRUCTURAL FORMULAS (703) BY PREDETERMINED METHOD
EXPERIMENTAL CONDITION (704)	CONDITION NUMERICAL VALUE OTHER THAN MATERIAL STRUCTURAL FORMULA
...	
FEATURE VALUES ABOUT TASK [1] (1202)	FEATURE VALUES GENERATED USING MODEL RELATED TO FIRST OTHER TASK
FEATURE VALUES ABOUT TASK [2] (1203)	FEATURE VALUES GENERATED USING MODEL RELATED TO SECOND OTHER TASK
...	...